



STIC SEARCH RESULTS FEEDBACK FORM

Biotech-Chem Library

Questions about the scope or the results of the search? Contact ***the searcher or contact:***

Mary Hale, Information Branch Supervisor
Remsen Bldg. 01 D86
571-272-2507

Voluntary Results Feedback Form

➤ I am an examiner in Workgroup: Example: 1610

➤ Relevant prior art **found**, search results used as follows:

- ☐ 102 rejection
- ☐ 103 rejection
- ☐ Cited as being of interest.
- ☐ Helped examiner better understand the invention.
- ☐ Helped examiner better understand the state of the art in their technology.

Types of relevant prior art found:

- ☐ Foreign Patent(s)
- ☐ Non-Patent Literature
(journal articles, conference proceedings, new product announcements etc.)

➤ Relevant prior art **not found**:

- ☐ Results verified the lack of relevant prior art (helped determine patentability).
- ☐ Results were not useful in determining patentability or understanding the invention.

Comments:

Drop off or send completed forms to STIC-Biotech-Chem Library Remsen Bldg.



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PLEASE PRINT CLEARLY

5.3.06

Scientific and Technical Information Center

SEARCH REQUEST FORM

Requester's Full Name: Perley (Robert) Shaw Examiner #: 79521 Date: 4/12/06
Art Unit: 1626 Phone Number: 2-0707 Serial Number: 10/734,208
Location (Bldg/Room#): REM (Mailbox #): 5A101 Results Format Preferred (circle): PAPER DISK
*****15218*****

To ensure an efficient and quality search, please attach a copy of the cover sheet, claims, and abstract or fill out the following:

Title of Invention: Synthesis of mono-N-substituted
Inventors (please provide full names): Selva et al

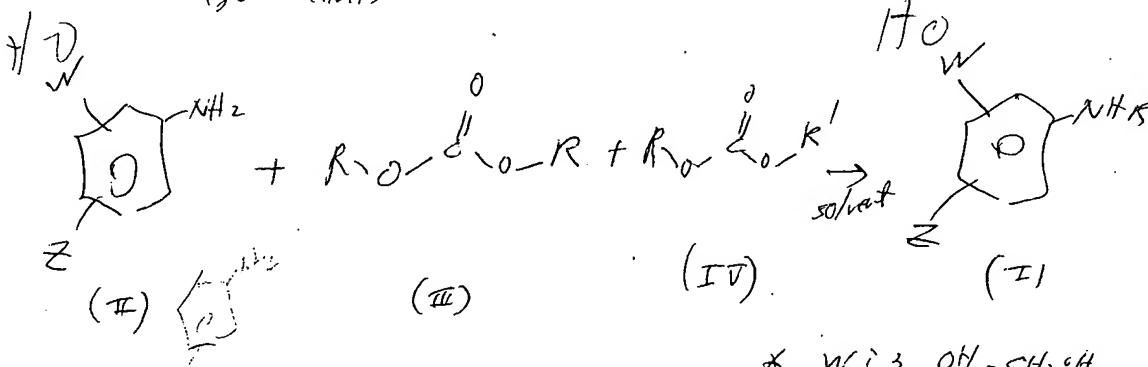
Earliest Priority Date: _____

Search Topic:

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc., if known.

For Sequence Searches Only Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.

Z seep a proced making compd by
(see claim 1)



* W is OH, -CH₂OH,
-COOH, -CONH₂

* Z is H, halogen,
alkyl, alkoxy, NO₂,
-CN

* R is alkyl

* R' is CH₂(OCH₂CH₂)_n, n = 2
or alkyl

STAFF USE ONLY

Searcher: _____

Searcher Phone #: _____

Searcher Location: _____

Date Searcher Picked Up: _____

Date Completed: _____

Searcher Prep & Review Time: _____

Online Time: _____

Type of Search

____ NA Sequence (#)

____ AA Sequence (#)

____ Structure (#)

____ Bibliographic

____ Litigation

____ Fulltext

____ Other

Vendors and cost where applicable

____ STN _____ Dialog

____ Questel/Orbit _____ Lexis/Nexis

____ Westlaw _____ WWW/Internet

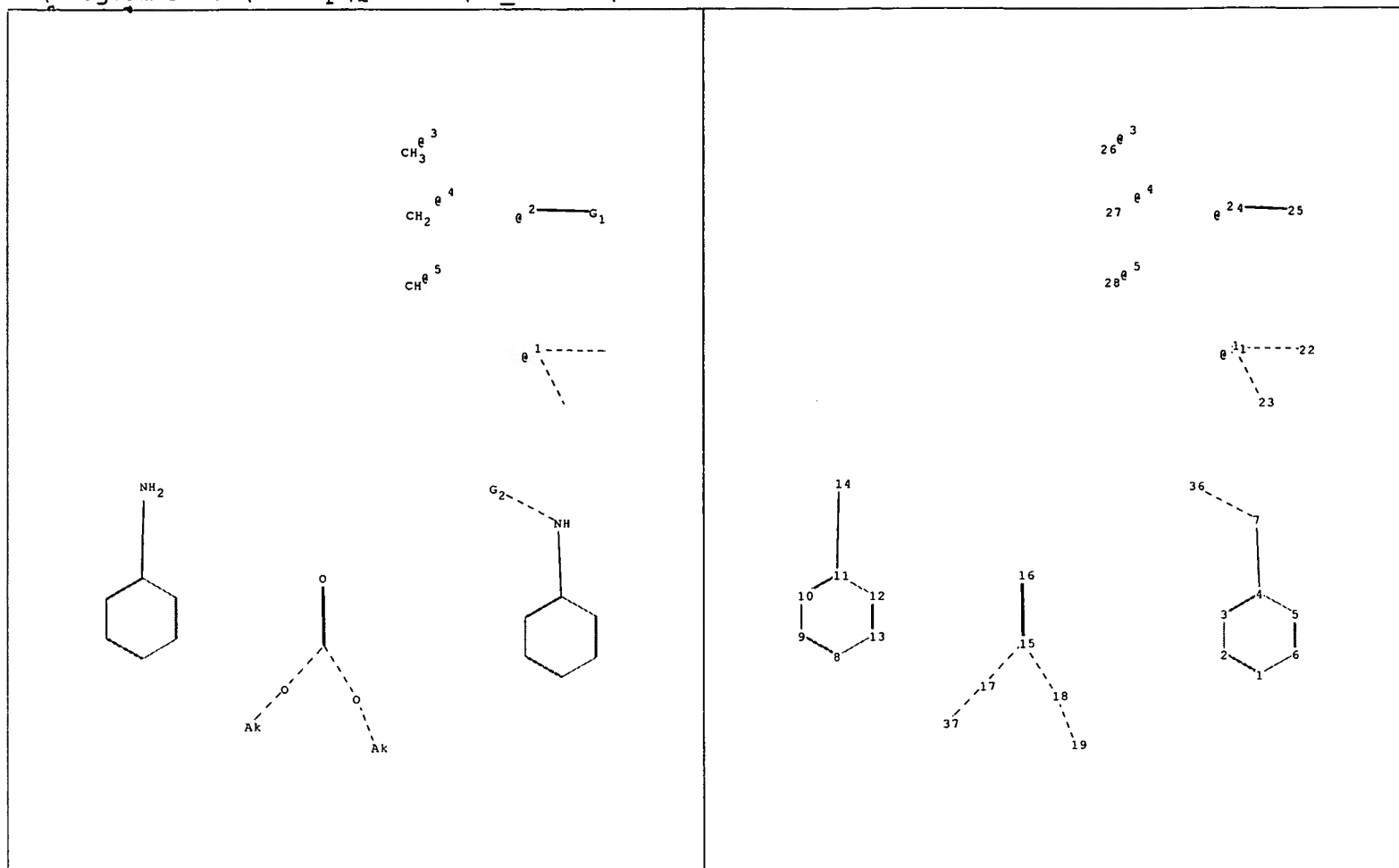
____ In-house sequence systems

____ Commercial _____ Oligomer _____ Score/Length

____ Interference _____ SPDI _____ Encode/Transl

____ Other (specify)

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chain nodes :

7 14 15 16 17 18 19 21 22 23 24 25 26 27 28 36 37

ring nodes :

1 2 3 4 5 6 8 9 10 11 12 13

chain bonds :

4-7 7-36 11-14 15-16 15-17 15-18 17-37 18-19 21-22 21-23 24-25

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 8-9 8-13 9-10 10-11 11-12 12-13

exact/norm bonds :

4-7 7-36 11-14 15-16 15-17 15-18 17-37 18-19 21-22 21-23 24-25

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 8-9 8-13 9-10 10-11 11-12 12-13

isolated ring systems :

containing 1 : 8 :

G1:C,N

G2:[*1],[*2],[*3],[*4],[*5]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:Atom 9:Atom 10:Atom 11:Atom

12:Atom 13:Atom 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS 21:CLASS

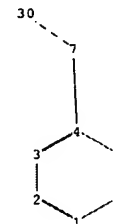
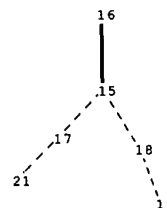
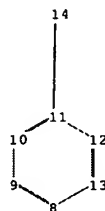
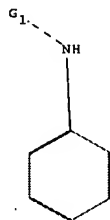
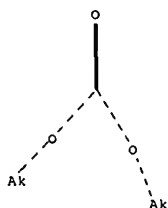
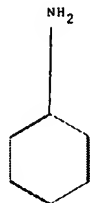
22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS 36:CLASS 37:CLASS

fragments assigned product role:

containing 1

fragments assigned reactant/reagent role:

containing 8
containing 15

Ak¹e²k-----Cb23¹e²3-----26

chain nodes :

7 14 15 16 17 18 19 21 23 25 26 30

ring nodes :

1 2 3 4 5 6 8 9 10 11 12 13

chain bonds :

4-7 7-30 11-14 15-16 15-17 15-18 17-21 18-19 25-26

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 8-9 8-13 9-10 10-11 11-12 12-13

exact/norm bonds :

4-7 7-30 11-14 15-16 15-17 15-18 17-21 18-19 25-26

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 8-9 8-13 9-10 10-11 11-12 12-13

isolated ring systems :

containing 1 : 8 :

G1:[*1],[*2]

Connectivity :

23:1 E exact RC ring/chain 25:2 E exact RC ring/chain

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:Atom 9:Atom 10:Atom 11:Atom

12:Atom 13:Atom 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS 21:CLASS

23:CLASS 25:CLASS 26:Atom 30:CLASS

fragments assigned product role:

containing 1

fragments assigned reactant/reagent role:

containing 8
containing 15

Search history

Shiao 10/734208

05/03/2006

=> d his full

(FILE 'HOME' ENTERED AT 15:22:57 ON 03 MAY 2006)

FILE 'STNGUIDE' ENTERED AT 15:23:28 ON 03 MAY 2006

FILE 'CASREACT' ENTERED AT 15:28:35 ON 03 MAY 2006

L1 STRUCTURE UPLOADED
L2 12 SEA SSS SAM L1 (65 REACTIONS)

FILE 'CAPLUS' ENTERED AT 15:29:02 ON 03 MAY 2006

L3 1 SEA ABB=ON PLU=ON US2003-734208/AP
SEL RN

FILE 'REGISTRY' ENTERED AT 15:29:24 ON 03 MAY 2006

L4 32 SEA ABB=ON PLU=ON (105-58-8/BI OR 10541-83-0/BI OR 110-71-4/B
I OR 112-49-2/BI OR 118-92-3/BI OR 119-68-6/BI OR 123-30-8/BI
OR 141814-27-9/BI OR 14703-69-6/BI OR 150-13-0/BI OR 150-75-4/B
I OR 15022-08-9/BI OR 17318-49-9/BI OR 181819-75-0/BI OR
214470-03-8/BI OR 2835-68-9/BI OR 29055-08-1/BI OR 3459-92-5/BI
OR 35472-56-1/BI OR 38359-26-1/BI OR 5344-90-1/BI OR 591-27-5/
BI OR 611-24-5/BI OR 616-38-6/BI OR 623-04-1/BI OR 7440-23-5/BI
OR 7440-37-1/BI OR 7505-81-9/BI OR 7727-37-9/BI OR 88-68-6/BI
OR 89-50-9/BI OR 95-55-6/BI)

FILE 'CASREACT' ENTERED AT 15:29:38 ON 03 MAY 2006

L5 STRUCTURE UPLOADED
L6 6 SEA SSS SAM L5 (6 REACTIONS)

FILE 'REGISTRY' ENTERED AT 15:30:18 ON 03 MAY 2006

L7 6 SEA ABB=ON PLU=ON FAUJASIT?

FILE 'CAPLUS' ENTERED AT 15:30:29 ON 03 MAY 2006

L8 3769 SEA ABB=ON PLU=ON FAUJASIT?/OBI

FILE 'REGISTRY' ENTERED AT 15:30:44 ON 03 MAY 2006

L9 1 SEA ABB=ON PLU=ON ANILINE/CN

FILE 'CAPLUS' ENTERED AT 15:30:56 ON 03 MAY 2006

L10 49252 SEA ABB=ON PLU=ON L9
L11 23 SEA ABB=ON PLU=ON L8 AND L10
L12 25354 SEA ABB=ON PLU=ON L9 (L) (RCT OR RGT OR RACT)/RL
L13 16 SEA ABB=ON PLU=ON L8 AND L12
SEL RN L11

FILE 'REGISTRY' ENTERED AT 15:36:53 ON 03 MAY 2006

L14 297 SEA ABB=ON PLU=ON (62-53-3/BI OR 1335-30-4/BI OR 100-61-8/BI
OR 106-49-0/BI OR 121-69-7/BI OR 104-94-9/BI OR 95-53-4/BI OR
100-01-6/BI OR 106-47-8/BI OR 108-95-2/BI OR 616-38-6/BI OR
7631-86-9/BI OR 100-15-2/BI OR 108-44-1/BI OR 108-88-3/BI OR
1314-23-4/BI OR 1330-20-7/BI OR 1344-28-1/BI OR 67-56-1/BI OR
71-43-2/BI OR 99-97-8/BI OR 100-23-2/BI OR 100-41-4/BI OR
100-46-9/BI OR 101-77-9/BI OR 101-81-5/BI OR 103-32-2/BI OR
103-69-5/BI OR 108-67-8/BI OR 110-86-1/BI OR 12173-28-3/BI OR
12173-98-7/BI OR 1309-48-4/BI OR 1314-35-8/BI OR 13463-67-7/BI
OR 141814-27-9/BI OR 150-13-0/BI OR 23713-49-7/BI OR 3459-92-5/
BI OR 50-00-0/BI OR 588-59-0/BI OR 589-16-2/BI OR 5961-59-1/BI
OR 623-08-5/BI OR 643-28-7/BI OR 67-63-0/BI OR 7440-05-3/BI OR
7440-06-4/BI OR 7440-50-8/BI OR 90-04-0/BI OR 932-96-7/BI OR
98-82-8/BI OR 98-95-3/BI OR 100-00-5/BI OR 100-17-4/BI OR

100-42-5/BI OR 100-44-7/BI OR 100-47-0/BI OR 100-66-3/BI OR
10072-05-6/BI OR 102-07-8/BI OR 103-29-7/BI OR 103-65-1/BI OR
103-67-3/BI OR 103-73-1/BI OR 103-83-3/BI OR 104-13-2/BI OR
104-76-7/BI OR 10402-24-1/BI OR 105-05-5/BI OR 105-58-8/BI OR
10541-83-0/BI OR 106-42-3/BI OR 106-44-5/BI OR 106-98-9/BI OR
108-38-3/BI OR 108-39-4/BI OR 108-45-2/BI OR 108-47-4/BI OR
108-48-5/BI OR 108-89-4/BI OR 108-99-6/BI OR 109-06-8/BI OR
109-75-1/BI OR 110-54-3/BI OR 110-82-7/BI OR 11098-99-0/BI OR
11099-11-9/BI OR 111-77-3/BI OR 11116-47-5/BI OR 11118-57-3/BI
OR 112-49-2/BI OR 112-62-9/BI OR 115-07-1/BI OR 115-11-7/BI OR
119-61-9/BI OR 119-65-3/BI OR 1197-19-9/BI OR 120-12-7/BI OR
121-44-8/BI OR 1219-99-4/BI OR 122-39-4/BI OR 1227-44-7/BI OR
12417-81-1/BI OR 12510-42-8/BI OR 12627-00-8/BI OR 12737-86-9/B
I OR 129-00-0/BI OR 1300-71-6/BI OR 1300-73-8/BI OR 1302-42-7/B
I OR 1303-86-2/BI OR 1305-78-8/BI OR 1308-38-9/BI OR 1310-73-2/
BI OR 1311-10-0/BI OR

FILE 'CAPLUS' ENTERED AT 15:37:35 ON 03 MAY 2006

L15 310569 SEA ABB=ON PLU=ON L14/P
L16 310605 SEA ABB=ON PLU=ON L14/PREP
L17 20 SEA ABB=ON PLU=ON L16 AND L11
L18 447798 SEA ABB=ON PLU=ON ?CARBONAT?/BI
L19 6 SEA ABB=ON PLU=ON L11 AND L18
SEL HIT RN
SEL HIT RN L17

FILE 'REGISTRY' ENTERED AT 15:39:07 ON 03 MAY 2006

L20 80 SEA ABB=ON PLU=ON (62-53-3/BI OR 100-61-8/BI OR 121-69-7/BI
OR 100-15-2/BI OR 106-49-0/BI OR 95-53-4/BI OR 100-23-2/BI OR
101-77-9/BI OR 103-32-2/BI OR 103-69-5/BI OR 643-28-7/BI OR
932-96-7/BI OR 99-97-8/BI OR 100-41-4/BI OR 10072-05-6/BI OR
101-81-5/BI OR 102-07-8/BI OR 103-29-7/BI OR 104-94-9/BI OR
10541-83-0/BI OR 106-47-8/BI OR 108-44-1/BI OR 108-45-2/BI OR
108-47-4/BI OR 108-48-5/BI OR 108-99-6/BI OR 109-06-8/BI OR
1197-19-9/BI OR 1219-99-4/BI OR 122-39-4/BI OR 1227-44-7/BI OR
1300-73-8/BI OR 13519-75-0/BI OR 13519-80-7/BI OR 14309-92-3/BI
OR 150-13-0/BI OR 1943-87-9/BI OR 20642-93-7/BI OR 214470-03-8
/BI OR 21911-84-2/BI OR 23574-01-8/BI OR 24007-66-7/BI OR
24544-04-5/BI OR 2603-10-3/BI OR 28685-60-1/BI OR 2948-37-0/BI
OR 30438-94-9/BI OR 30448-32-9/BI OR 329767-78-4/BI OR
3665-80-3/BI OR 40871-06-5/BI OR 4138-15-2/BI OR 4138-40-3/BI
OR 42313-52-0/BI OR 4714-62-9/BI OR 53733-94-1/BI OR 56525-67-8
/BI OR 589-09-3/BI OR 5961-59-1/BI OR 611-21-2/BI OR 620-50-8/B
I OR 621-00-1/BI OR 622-14-0/BI OR 623-08-5/BI OR 698-69-1/BI
OR 7143-42-2/BI OR 74-90-8/BI OR 767-71-5/BI OR 768-52-5/BI OR
769-06-2/BI OR 793-19-1/BI OR 85-91-6/BI OR 864377-09-3/BI OR
90-04-0/BI OR 91-66-7/BI OR 91-73-6/BI OR 94563-11-8/BI OR
95-51-2/BI OR 95-55-6/BI OR 99-88-7/BI)

FILE 'CAPLUS' ENTERED AT 15:39:42 ON 03 MAY 2006

SEL RN L13

FILE 'REGISTRY' ENTERED AT 15:39:51 ON 03 MAY 2006

L21 218 SEA ABB=ON PLU=ON (1335-30-4/BI OR 62-53-3/BI OR 100-61-8/BI
OR 106-49-0/BI OR 121-69-7/BI OR 100-01-6/BI OR 104-94-9/BI OR
106-47-8/BI OR 616-38-6/BI OR 95-53-4/BI OR 100-15-2/BI OR
7631-86-9/BI OR 99-97-8/BI OR 100-23-2/BI OR 100-46-9/BI OR
101-77-9/BI OR 103-32-2/BI OR 108-44-1/BI OR 108-88-3/BI OR
110-86-1/BI OR 1309-48-4/BI OR 1314-23-4/BI OR 1314-35-8/BI OR
1330-20-7/BI OR 1344-28-1/BI OR 13463-67-7/BI OR 141814-27-9/BI)

OR 3459-92-5/BI OR 50-00-0/BI OR 589-16-2/BI OR 5961-59-1/BI
OR 623-08-5/BI OR 643-28-7/BI OR 67-56-1/BI OR 71-43-2/BI OR
7440-05-3/BI OR 7440-06-4/BI OR 7440-50-8/BI OR 932-96-7/BI OR
100-41-4/BI OR 100-44-7/BI OR 100-47-0/BI OR 100-66-3/BI OR
10072-05-6/BI OR 101-81-5/BI OR 102-07-8/BI OR 103-65-1/BI OR
103-67-3/BI OR 103-69-5/BI OR 103-73-1/BI OR 103-83-3/BI OR
104-13-2/BI OR 10402-24-1/BI OR 105-05-5/BI OR 105-58-8/BI OR
10541-83-0/BI OR 106-42-3/BI OR 106-44-5/BI OR 106-98-9/BI OR
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108-95-2/BI OR 109-75-1/BI OR 110-54-3/BI OR 110-82-7/BI OR
11098-99-0/BI OR 11099-11-9/BI OR 111-77-3/BI OR 11118-57-3/BI
OR 112-49-2/BI OR 115-07-1/BI OR 115-11-7/BI OR 119-65-3/BI OR
1197-19-9/BI OR 120-12-7/BI OR 121-44-8/BI OR 12173-28-3/BI OR
12173-98-7/BI OR 1219-99-4/BI OR 1227-44-7/BI OR 12627-00-8/BI
OR 129-00-0/BI OR 1300-71-6/BI OR 1300-73-8/BI OR 1302-42-7/BI
OR 1303-86-2/BI OR 1305-78-8/BI OR 1308-38-9/BI OR 1310-73-2/BI
OR 1311-10-0/BI OR 1314-13-2/BI OR 1314-56-3/BI OR 1314-62-1/BI
OR 13308-51-5/BI OR 1333-41-1/BI OR 13330-29-5/BI OR
1345-13-7/BI OR 135-01-3/BI OR 13519-75-0/BI OR 13519-80-7/BI
OR 137273-36-0/BI OR 13765-95-2/BI OR 13765-96-3/BI OR
141-93-5/BI OR 141-97-9/BI OR 14309-92-3/BI OR 14414-90-5/BI
OR 150-13-0/BI OR 15022-08-9/BI OR 156-43-4/BI OR 1864-93-3/BI
OR 18707-60-3/BI OR 1943-8

FILE 'CAPLUS' ENTERED AT 15:40:21 ON 03 MAY 2006

L22 227422 SEA ABB=ON PLU=ON L21/PREP
L23 14 SEA ABB=ON PLU=ON L22 AND L13
SEL HIT RN

FILE 'REGISTRY' ENTERED AT 15:40:55 ON 03 MAY 2006

L24 63 SEA ABB=ON PLU=ON (62-53-3/BI OR 100-61-8/BI OR 121-69-7/BI
OR 100-15-2/BI OR 100-23-2/BI OR 101-77-9/BI OR 103-32-2/BI OR
106-49-0/BI OR 643-28-7/BI OR 932-96-7/BI OR 95-53-4/BI OR
99-97-8/BI OR 10072-05-6/BI OR 102-07-8/BI OR 103-69-5/BI OR
10541-83-0/BI OR 1197-19-9/BI OR 1219-99-4/BI OR 1227-44-7/BI
OR 1300-73-8/BI OR 13519-75-0/BI OR 13519-80-7/BI OR 14309-92-3/
/BI OR 1943-87-9/BI OR 20642-93-7/BI OR 214470-03-8/BI OR
21911-84-2/BI OR 23574-01-8/BI OR 24007-66-7/BI OR 24544-04-5/B
I OR 2603-10-3/BI OR 28685-60-1/BI OR 2948-37-0/BI OR 30438-94-
9/BI OR 30448-32-9/BI OR 329767-78-4/BI OR 3665-80-3/BI OR
40871-06-5/BI OR 4138-15-2/BI OR 4138-40-3/BI OR 42313-52-0/BI
OR 4714-62-9/BI OR 53733-94-1/BI OR 56525-67-8/BI OR 589-09-3/B
I OR 5961-59-1/BI OR 611-21-2/BI OR 620-50-8/BI OR 621-00-1/BI
OR 622-14-0/BI OR 623-08-5/BI OR 698-69-1/BI OR 7143-42-2/BI
OR 74-90-8/BI OR 767-71-5/BI OR 768-52-5/BI OR 769-06-2/BI OR
793-19-1/BI OR 85-91-6/BI OR 864377-09-3/BI OR 91-73-6/BI OR
94563-11-8/BI OR 99-88-7/BI)

FILE 'CAPLUS' ENTERED AT 15:41:16 ON 03 MAY 2006

L25 4 SEA ABB=ON PLU=ON L23 AND L19
L26 5 SEA ABB=ON PLU=ON L17 AND L19
L27 5 SEA ABB=ON PLU=ON (L25 OR L26)

FILE 'CASREACT' ENTERED AT 15:41:45 ON 03 MAY 2006

L28 6 SEA SSS SAM L5 (6 REACTIONS)
L29 91 SEA SSS FUL L5 (702 REACTIONS)
L30 179 SEA ABB=ON PLU=ON FAUJASIT?
L31 5 SEA ABB=ON PLU=ON L29 AND L30

FILE 'CAPLUS' ENTERED AT 15:42:39 ON 03 MAY 2006

L32 5 SEA ABB=ON PLU=ON L31
L33 2 SEA ABB=ON PLU=ON L19 AND L32

FILE 'CASREACT' ENTERED AT 15:42:57 ON 03 MAY 2006

L34 STRUCTURE UPLOADED
L35 4 SEA SUB=L29 SSS SAM L34 (4 REACTIONS)
L36 48 SEA SUB=L29 SSS FUL L34 (243 REACTIONS)
L37 32 SEA ABB=ON PLU=ON SELVA M?/AU
L38 57 SEA ABB=ON PLU=ON TUNDO P?/AU
L39 7 SEA ABB=ON PLU=ON L36 AND (L37 OR L38)

FILE 'CAPLUS' ENTERED AT 15:44:21 ON 03 MAY 2006

L40 70 SEA ABB=ON PLU=ON SELVA M?/AU
L41 196 SEA ABB=ON PLU=ON TUNDO P?/AU
L42 62 SEA ABB=ON PLU=ON L40 AND L41
L43 3 SEA ABB=ON PLU=ON (L40 OR L41) AND (L19 OR L25 OR L26)
L44 3 SEA ABB=ON PLU=ON (L40 OR L41) AND (L13 OR L23)
L45 48 SEA ABB=ON PLU=ON L36
L46 5 SEA ABB=ON PLU=ON L8 AND L45
L47 5 SEA ABB=ON PLU=ON L32 AND L46
L48 5 SEA ABB=ON PLU=ON L30 AND L36

FILE 'CASREACT' ENTERED AT 15:46:19 ON 03 MAY 2006

L49 48 SEA ABB=ON PLU=ON L31 OR L36 OR L48
L50 41 SEA ABB=ON PLU=ON L49 NOT L39

FILE 'CAPLUS' ENTERED AT 15:47:01 ON 03 MAY 2006

L51 86 SEA ABB=ON PLU=ON L18 AND L8
L52 6 SEA ABB=ON PLU=ON L51 AND L10
L53 9721 SEA ABB=ON PLU=ON AMINES/CT (L) AROMATIC/OBI
L54 5 SEA ABB=ON PLU=ON L51 AND L53
L55 3 SEA ABB=ON PLU=ON L52 AND L54
L56 8 SEA ABB=ON PLU=ON L19 OR L25 OR L26 OR L54 OR L55
L57 4 SEA ABB=ON PLU=ON (L40 OR L41) AND L56

FILE 'CASREACT' ENTERED AT 15:50:07 ON 03 MAY 2006

D STAT QUE L31
D STAT QUE L36
D QUE NOS L48
L58 41 SEA ABB=ON PLU=ON (L31 OR L36 OR L48) NOT L39

FILE 'REGISTRY' ENTERED AT 15:51:42 ON 03 MAY 2006

FILE 'CAPLUS' ENTERED AT 15:51:46 ON 03 MAY 2006

D STAT QUE L19
D STAT QUE L25
D STAT QUE L26
D STAT QUE L54
D STAT QUE L54
D STAT QUE L55
L59 4 SEA ABB=ON PLU=ON (L19 OR L25 OR L26 OR L54 OR L55) NOT L57

FILE 'CASREACT, CAPLUS' ENTERED AT 15:54:05 ON 03 MAY 2006

L60 44 DUP REM L58 L59 (1 DUPLICATE REMOVED)
ANSWERS '1-41' FROM FILE CASREACT
ANSWERS '42-44' FROM FILE CAPLUS
D IBIB ABS HIT L60 1-41
D IBIB ABS HITIND HITSTR L60 42-44

FILE 'CASREACT' ENTERED AT 16:00:03 ON 03 MAY 2006

D STAT QUE L39

FILE 'CAPLUS' ENTERED AT 16:00:22 ON 03 MAY 2006
D STAT QUE L57

L61 FILE 'CASREACT, CAPLUS' ENTERED AT 16:00:38 ON 03 MAY 2006
9 DUP REM L39 L57 (2 DUPLICATES REMOVED)
ANSWERS '1-7' FROM FILE CASREACT
ANSWERS '8-9' FROM FILE CAPLUS
D IBIB ABS HIT L61 1-7
D IBIB ABS HITIND HITSTR L61 8-9

FILE HOME

FILE STNGUIDE
FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: May 2, 2006 (20060502/UP).

FILE CASREACT
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FILE CONTENT:1840 - 30 Apr 2006 VOL 144 ISS 18

New CAS Information Use Policies, enter HELP USAGETERMS for details.

*
* CASREACT now has more than 10 million reactions *
*

Some CASREACT records are derived from the ZIC/VINITI database (1974-1991) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance identification.

FILE CAPLUS

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FILE COVERS 1907 - 3 May 2006 VOL 144 ISS 19
FILE LAST UPDATED: 2 May 2006 (20060502/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

<http://www.cas.org/infopolicy.html>

FILE REGISTRY

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 2 MAY 2006 HIGHEST RN 882569-16-6

DICTIONARY FILE UPDATES: 2 MAY 2006 HIGHEST RN 882569-16-6

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 6, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

```
*****
*
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added,   *
* effective March 20, 2005. A new display format, IDERL, is now      *
* available and contains the CA role and document type information.  *
*
*****
```

Structure search iteration limits have been increased. See HELP SLIMITS for details.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

=>

=> file casreact

FILE 'CASREACT' ENTERED AT 15:50:07 ON 03 MAY 2006
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CASREACT
SEARCH

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FILE CONTENT:1840 - 30 Apr 2006 VOL 144 ISS 18

New CAS Information Use Policies, enter HELP USAGETERMS for details.

*
* CASREACT now has more than 10 million reactions *
*

Some CASREACT records are derived from the ZIC/VINITI database (1974-1991) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

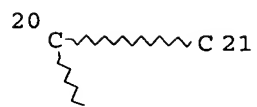
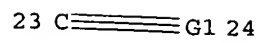
This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d stat que L31
L5 STR
C 30 N 31

25 C M3

26 C M2

27 C M1



Page 1-B

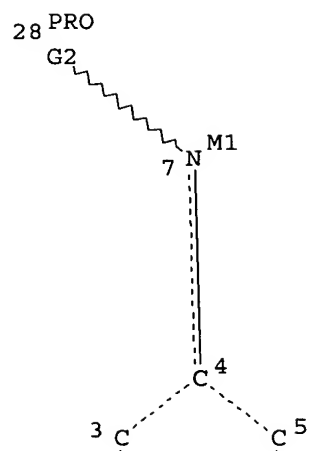
RRT



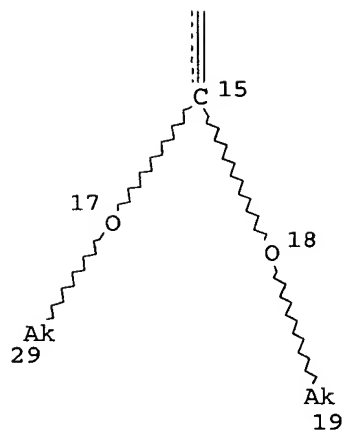
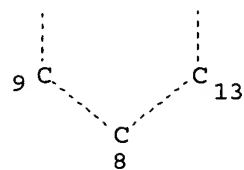
RRT



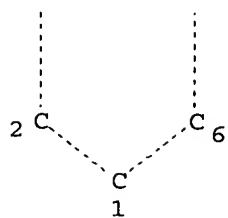
Page 2-A



Page 2-B



Page 3-A



Page 3-B

VAR G1=30/31

VAR G2=20/23/25/26/27

NODE ATTRIBUTES:

HCOUNT	IS	M1	AT	7
HCOUNT	IS	M2	AT	14
HCOUNT	IS	M3	AT	25
HCOUNT	IS	M2	AT	26
HCOUNT	IS	M1	AT	27
NSPEC	IS	R	AT	1
NSPEC	IS	R	AT	2
NSPEC	IS	R	AT	3
NSPEC	IS	R	AT	4
NSPEC	IS	R	AT	5
NSPEC	IS	R	AT	6
NSPEC	IS	C	AT	7
NSPEC	IS	R	AT	8
NSPEC	IS	R	AT	9
NSPEC	IS	R	AT	10
NSPEC	IS	R	AT	11
NSPEC	IS	R	AT	12
NSPEC	IS	R	AT	13
NSPEC	IS	C	AT	14
NSPEC	IS	C	AT	15
NSPEC	IS	C	AT	16
NSPEC	IS	C	AT	17
NSPEC	IS	C	AT	18
NSPEC	IS	C	AT	19
NSPEC	IS	C	AT	20
NSPEC	IS	C	AT	21
NSPEC	IS	C	AT	22
NSPEC	IS	C	AT	23
NSPEC	IS	C	AT	24
NSPEC	IS	C	AT	25
NSPEC	IS	C	AT	26
NSPEC	IS	C	AT	27
NSPEC	IS	C	AT	28
NSPEC	IS	C	AT	29

DEFAULT MLEVEL IS ATOM

MLEVEL IS CLASS AT 7 14 15 16 17 18 19 20 21 22 23 25 26 27 29 30 31

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RSPEC I

NUMBER OF NODES IS 31

STEREO ATTRIBUTES: NONE

L29 91 SEA FILE=CASREACT SSS FUL L5 (702 REACTIONS)

L30 179 SEA FILE=CASREACT ABB=ON PLU=ON FAUJASIT?

L31 5 SEA FILE=CASREACT ABB=ON PLU=ON L29 AND L30

=> d stat que L36

L5 STR

C 30 N 31

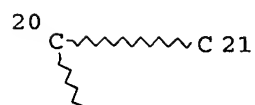
25 C M3

26 C M2

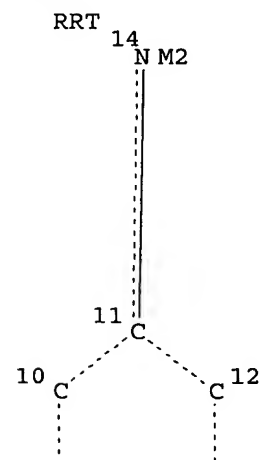
27 C M1

Page 1-A

23 C \equiv G1 24



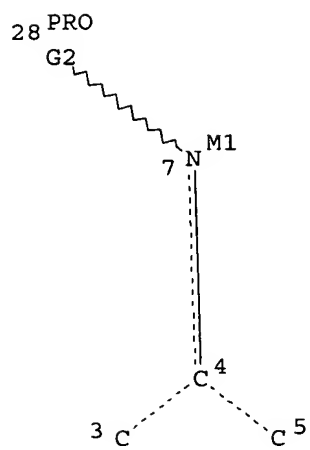
Page 1-B



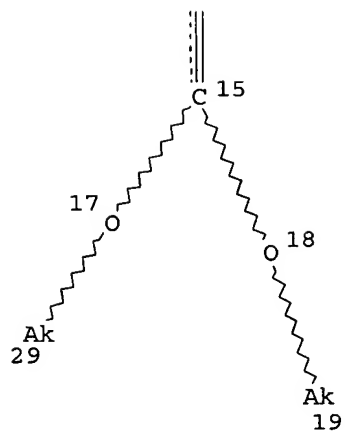
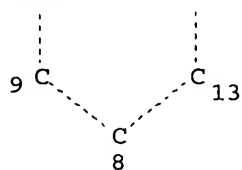
RRT



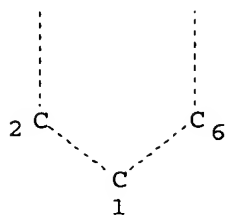
Page 2-A



Page 2-B



Page 3-A



Page 3-B

VAR G1=30/31

VAR G2=20/23/25/26/27

NODE ATTRIBUTES:

HCOUNT	IS	M1	AT	7
HCOUNT	IS	M2	AT	14
HCOUNT	IS	M3	AT	25
HCOUNT	IS	M2	AT	26
HCOUNT	IS	M1	AT	27
NSPEC	IS	R	AT	1
NSPEC	IS	R	AT	2
NSPEC	IS	R	AT	3
NSPEC	IS	R	AT	4
NSPEC	IS	R	AT	5
NSPEC	IS	R	AT	6
NSPEC	IS	C	AT	7
NSPEC	IS	R	AT	8
NSPEC	IS	R	AT	9
NSPEC	IS	R	AT	10
NSPEC	IS	R	AT	11
NSPEC	IS	R	AT	12
NSPEC	IS	R	AT	13
NSPEC	IS	C	AT	14
NSPEC	IS	C	AT	15
NSPEC	IS	C	AT	16
NSPEC	IS	C	AT	17
NSPEC	IS	C	AT	18
NSPEC	IS	C	AT	19
NSPEC	IS	C	AT	20
NSPEC	IS	C	AT	21
NSPEC	IS	C	AT	22
NSPEC	IS	C	AT	23
NSPEC	IS	C	AT	24
NSPEC	IS	C	AT	25
NSPEC	IS	C	AT	26
NSPEC	IS	C	AT	27
NSPEC	IS	C	AT	28
NSPEC	IS	C	AT	29

DEFAULT MLEVEL IS ATOM

MLEVEL IS CLASS AT 7 14 15 16 17 18 19 20 21 22 23 25 26 27 29 30 31

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RSPEC I

NUMBER OF NODES IS 31

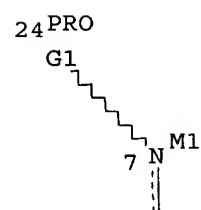
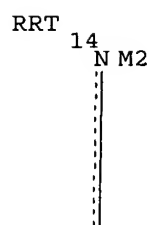
STEREO ATTRIBUTES: NONE

L29 91 SEA FILE=CASREACT SSS FUL L5 (702 REACTIONS)

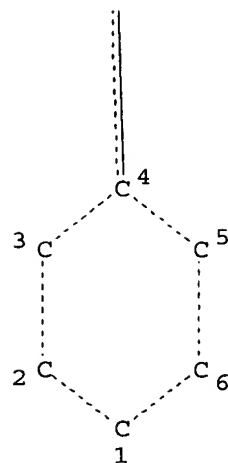
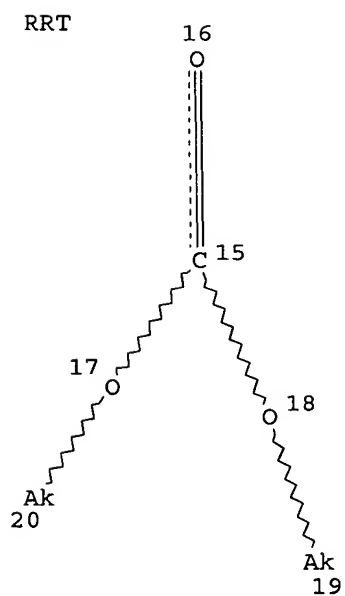
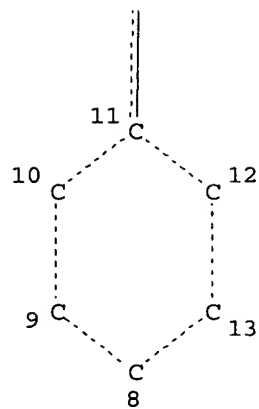
L34 STR

Ak 21

22 Ak~~~~~Cb 23



Page 1-A



Page 2-A
 VAR G1=21/22
 NODE ATTRIBUTES:

HCOUNT IS M1 AT 7
HCOUNT IS M2 AT 14
NSPEC IS R AT 1
NSPEC IS R AT 2
NSPEC IS R AT 3
NSPEC IS R AT 4
NSPEC IS R AT 5
NSPEC IS R AT 6
NSPEC IS C AT 7
NSPEC IS R AT 8
NSPEC IS R AT 9
NSPEC IS R AT 10
NSPEC IS R AT 11
NSPEC IS R AT 12
NSPEC IS R AT 13
NSPEC IS C AT 14
NSPEC IS C AT 15
NSPEC IS C AT 16
NSPEC IS C AT 17
NSPEC IS C AT 18
NSPEC IS C AT 19
NSPEC IS C AT 20
NSPEC IS C AT 21
NSPEC IS C AT 22
NSPEC IS C AT 23
NSPEC IS C AT 24
CONNECT IS E1 RC AT 21
CONNECT IS E2 RC AT 22
DEFAULT MLEVEL IS ATOM
MLEVEL IS CLASS AT 7 14 15 16 17 18 19 20 21 22
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RSPEC I

NUMBER OF NODES IS 24

STEREO ATTRIBUTES: NONE

L36 48 SEA FILE=CASREACT SUB=L29 SSS FUL L34 (243 REACTIONS)

100.0% DONE 702 VERIFIED 243 HIT RXNS 48 DOCS
SEARCH TIME: 00.00.01

=> d que nos L48

L5 STR

L29 91 SEA FILE=CASREACT SSS FUL L5 (702 REACTIONS)

L30 179 SEA FILE=CASREACT ABB=ON PLU=ON FAUJASIT?

L34 STR

L36 48 SEA FILE=CASREACT SUB=L29 SSS FUL L34 (243 REACTIONS)

L48 5 SEA FILE=CAPLUS ABB=ON PLU=ON L30 AND L36

=> s (L31 or L36 or L48) not L39

L58 41 (L31 OR L36 OR L48) NOT L39

printed with another search

=> file registry

FILE 'REGISTRY' ENTERED AT 15:51:42 ON 03 MAY 2006

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STRUCTURE FILE UPDATES: 2 MAY 2006 HIGHEST RN 882569-16-6

DICTIONARY FILE UPDATES: 2 MAY 2006 HIGHEST RN 882569-16-6

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 6, 2006

Please note that search-term pricing does apply when conducting SmartSELECT searches.

*
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added, *
* effective March 20, 2005. A new display format, IDERL, is now *
* available and contains the CA role and document type information. *
*

Structure search iteration limits have been increased. See HELP SLIMITS for details.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

=> file caplus

FILE 'CAPLUS' ENTERED AT 15:51:46 ON 03 MAY 2006

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CAPLUS
TEXT SEARCH

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FILE COVERS 1907 - 3 May 2006 VOL 144 ISS 19

FILE LAST UPDATED: 2 May 2006 (20060502/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

<http://www.cas.org/infopolicy.html>

'OBI' IS DEFAULT SEARCH FIELD FOR 'CAPLUS' FILE

=> d stat que L19

L8 3769 SEA FILE=CAPLUS ABB=ON PLU=ON FAUJASIT?/OBI
 L9 1 SEA FILE=REGISTRY ABB=ON PLU=ON ANILINE/CN
 L10 49252 SEA FILE=CAPLUS ABB=ON PLU=ON L9
 L11 23 SEA FILE=CAPLUS ABB=ON PLU=ON L8 AND L10
 L18 447798 SEA FILE=CAPLUS ABB=ON PLU=ON ?CARBONAT?/BI
 L19 6 SEA FILE=CAPLUS ABB=ON PLU=ON L11 AND L18

=> d stat que L25

L8 3769 SEA FILE=CAPLUS ABB=ON PLU=ON FAUJASIT?/OBI
 L9 1 SEA FILE=REGISTRY ABB=ON PLU=ON ANILINE/CN
 L10 49252 SEA FILE=CAPLUS ABB=ON PLU=ON L9
 L11 23 SEA FILE=CAPLUS ABB=ON PLU=ON L8 AND L10
 L12 25354 SEA FILE=CAPLUS ABB=ON PLU=ON L9 (L) (RCT OR RGT OR RACT)/RL

L13 16 SEA FILE=CAPLUS ABB=ON PLU=ON L8 AND L12
 L18 447798 SEA FILE=CAPLUS ABB=ON PLU=ON ?CARBONAT?/BI
 L19 6 SEA FILE=CAPLUS ABB=ON PLU=ON L11 AND L18
 L21 218 SEA FILE=REGISTRY ABB=ON PLU=ON (1335-30-4/BI OR 62-53-3/BI
 OR 100-61-8/BI OR 106-49-0/BI OR 121-69-7/BI OR 100-01-6/BI OR
 104-94-9/BI OR 106-47-8/BI OR 616-38-6/BI OR 95-53-4/BI OR
 100-15-2/BI OR 7631-86-9/BI OR 99-97-8/BI OR 100-23-2/BI OR
 100-46-9/BI OR 101-77-9/BI OR 103-32-2/BI OR 108-44-1/BI OR
 108-88-3/BI OR 110-86-1/BI OR 1309-48-4/BI OR 1314-23-4/BI OR
 1314-35-8/BI OR 1330-20-7/BI OR 1344-28-1/BI OR 13463-67-7/BI
 OR 141814-27-9/BI OR 3459-92-5/BI OR 50-00-0/BI OR 589-16-2/BI
 OR 5961-59-1/BI OR 623-08-5/BI OR 643-28-7/BI OR 67-56-1/BI OR
 71-43-2/BI OR 7440-05-3/BI OR 7440-06-4/BI OR 7440-50-8/BI OR
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 100-66-3/BI OR 10072-05-6/BI OR 101-81-5/BI OR 102-07-8/BI OR
 103-65-1/BI OR 103-67-3/BI OR 103-69-5/BI OR 103-73-1/BI OR
 103-83-3/BI OR 104-13-2/BI OR 10402-24-1/BI OR 105-05-5/BI OR
 105-58-8/BI OR 10541-83-0/BI OR 106-42-3/BI OR 106-44-5/BI OR
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 110-82-7/BI OR 11098-99-0/BI OR 11099-11-9/BI OR 111-77-3/BI
 OR 11118-57-3/BI OR 112-49-2/BI OR 115-07-1/BI OR 115-11-7/BI
 OR 119-65-3/BI OR 1197-19-9/BI OR 120-12-7/BI OR 121-44-8/BI
 OR 12173-28-3/BI OR 12173-98-7/BI OR 1219-99-4/BI OR 1227-44-7/
 BI OR 12627-00-8/BI OR 129-00-0/BI OR 1300-71-6/BI OR 1300-73-8
 /BI OR 1302-42-7/BI OR 1303-86-2/BI OR 1305-78-8/BI OR
 1308-38-9/BI OR 1310-73-2/BI OR 1311-10-0/BI OR 1314-13-2/BI
 OR 1314-56-3/BI OR 1314-62-1/BI OR 13308-51-5/BI OR 1333-41-1/B
 I OR 13330-29-5/BI OR 1345-13-7/BI OR 135-01-3/BI OR 13519-75-0
 /BI OR 13519-80-7/BI OR 137273-36-0/BI OR 13765-95-2/BI OR
 13765-96-3/BI OR 141-93-5/BI OR 141-97-9/BI OR 14309-92-3/BI
 OR 14414-90-5/BI OR 150-13-0/BI OR 15022-08-9/BI OR 156-43-4/BI
 OR 1864-93-3/BI OR 18707-60-3/BI OR 1943-8
 L22 227422 SEA FILE=CAPLUS ABB=ON PLU=ON L21/PREP
 L23 14 SEA FILE=CAPLUS ABB=ON PLU=ON L22 AND L13
 L25 4 SEA FILE=CAPLUS ABB=ON PLU=ON L23 AND L19

=> d stat que L26

L8 3769 SEA FILE=CAPLUS ABB=ON PLU=ON FAUJASIT?/OBI
 L9 1 SEA FILE=REGISTRY ABB=ON PLU=ON ANILINE/CN
 L10 49252 SEA FILE=CAPLUS ABB=ON PLU=ON L9
 L11 23 SEA FILE=CAPLUS ABB=ON PLU=ON L8 AND L10
 L14 297 SEA FILE=REGISTRY ABB=ON PLU=ON (62-53-3/BI OR 1335-30-4/BI

OR 100-61-8/BI OR 106-49-0/BI OR 121-69-7/BI OR 104-94-9/BI OR
 95-53-4/BI OR 100-01-6/BI OR 106-47-8/BI OR 108-95-2/BI OR
 616-38-6/BI OR 7631-86-9/BI OR 100-15-2/BI OR 108-44-1/BI OR
 108-88-3/BI OR 1314-23-4/BI OR 1330-20-7/BI OR 1344-28-1/BI OR
 67-56-1/BI OR 71-43-2/BI OR 99-97-8/BI OR 100-23-2/BI OR
 100-41-4/BI OR 100-46-9/BI OR 101-77-9/BI OR 101-81-5/BI OR
 103-32-2/BI OR 103-69-5/BI OR 108-67-8/BI OR 110-86-1/BI OR
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 OR 13463-67-7/BI OR 141814-27-9/BI OR 150-13-0/BI OR 23713-49-7
 /BI OR 3459-92-5/BI OR 50-00-0/BI OR 588-59-0/BI OR 589-16-2/BI
 OR 5961-59-1/BI OR 623-08-5/BI OR 643-28-7/BI OR 67-63-0/BI
 OR 7440-05-3/BI OR 7440-06-4/BI OR 7440-50-8/BI OR 90-04-0/BI
 OR 932-96-7/BI OR 98-82-8/BI OR 98-95-3/BI OR 100-00-5/BI OR
 100-17-4/BI OR 100-42-5/BI OR 100-44-7/BI OR 100-47-0/BI OR
 100-66-3/BI OR 10072-05-6/BI OR 102-07-8/BI OR 103-29-7/BI OR
 103-65-1/BI OR 103-67-3/BI OR 103-73-1/BI OR 103-83-3/BI OR
 104-13-2/BI OR 104-76-7/BI OR 10402-24-1/BI OR 105-05-5/BI OR
 105-58-8/BI OR 10541-83-0/BI OR 106-42-3/BI OR 106-44-5/BI OR
 106-98-9/BI OR 108-38-3/BI OR 108-39-4/BI OR 108-45-2/BI OR
 108-47-4/BI OR 108-48-5/BI OR 108-89-4/BI OR 108-99-6/BI OR
 109-06-8/BI OR 109-75-1/BI OR 110-54-3/BI OR 110-82-7/BI OR
 11098-99-0/BI OR 11099-11-9/BI OR 111-77-3/BI OR 11116-47-5/BI
 OR 11118-57-3/BI OR 112-49-2/BI OR 112-62-9/BI OR 115-07-1/BI
 OR 115-11-7/BI OR 119-61-9/BI OR 119-65-3/BI OR 1197-19-9/BI
 OR 120-12-7/BI OR 121-44-8/BI OR 1219-99-4/BI OR 122-39-4/BI
 OR 1227-44-7/BI OR 12417-81-1/BI OR 12510-42-8/BI OR 12627-00-8
 /BI OR 12737-86-9/BI OR 129-00-0/BI OR 1300-71-6/BI OR
 1300-73-8/BI OR 1302-42-7/BI OR 1303-86-2/BI OR 1305-78-8/BI
 OR 1308-38-9/BI OR 1310-73-2/BI OR 1311-10-0/BI OR

L16 310605 SEA FILE=CAPLUS ABB=ON PLU=ON L14/PREP
 L17 20 SEA FILE=CAPLUS ABB=ON PLU=ON L16 AND L11
 L18 447798 SEA FILE=CAPLUS ABB=ON PLU=ON ?CARBONAT?/BI
 L19 6 SEA FILE=CAPLUS ABB=ON PLU=ON L11 AND L18
 L26 5 SEA FILE=CAPLUS ABB=ON PLU=ON L17 AND L19

=> d stat que L54

L8 3769 SEA FILE=CAPLUS ABB=ON PLU=ON FAUJASIT?/OBI
 L18 447798 SEA FILE=CAPLUS ABB=ON PLU=ON ?CARBONAT?/BI
 L51 86 SEA FILE=CAPLUS ABB=ON PLU=ON L18 AND L8
 L53 9721 SEA FILE=CAPLUS ABB=ON PLU=ON AMINES/CT (L) AROMATIC/OBI
 L54 5 SEA FILE=CAPLUS ABB=ON PLU=ON L51 AND L53

=> d stat que L54

L8 3769 SEA FILE=CAPLUS ABB=ON PLU=ON FAUJASIT?/OBI
 L18 447798 SEA FILE=CAPLUS ABB=ON PLU=ON ?CARBONAT?/BI
 L51 86 SEA FILE=CAPLUS ABB=ON PLU=ON L18 AND L8
 L53 9721 SEA FILE=CAPLUS ABB=ON PLU=ON AMINES/CT (L) AROMATIC/OBI
 L54 5 SEA FILE=CAPLUS ABB=ON PLU=ON L51 AND L53

=> d stat que L55

L8 3769 SEA FILE=CAPLUS ABB=ON PLU=ON FAUJASIT?/OBI
 L9 1 SEA FILE=REGISTRY ABB=ON PLU=ON ANILINE/CN
 L10 49252 SEA FILE=CAPLUS ABB=ON PLU=ON L9
 L18 447798 SEA FILE=CAPLUS ABB=ON PLU=ON ?CARBONAT?/BI
 L51 86 SEA FILE=CAPLUS ABB=ON PLU=ON L18 AND L8
 L52 6 SEA FILE=CAPLUS ABB=ON PLU=ON L51 AND L10
 L53 9721 SEA FILE=CAPLUS ABB=ON PLU=ON AMINES/CT (L) AROMATIC/OBI

L54 5 SEA FILE=CAPLUS ABB=ON PLU=ON L51 AND L53
 L55 3 SEA FILE=CAPLUS ABB=ON PLU=ON L52 AND L54

=> s (L19 or L25 or L26 or L54 or L55) not L57

L59 4 (L19 OR L25 OR L26 OR L54 OR L55) NOT L57

*printed
with
author search*

=> dup rem L58 L59

FILE 'CASREACT' ENTERED AT 15:54:05 ON 03 MAY 2006
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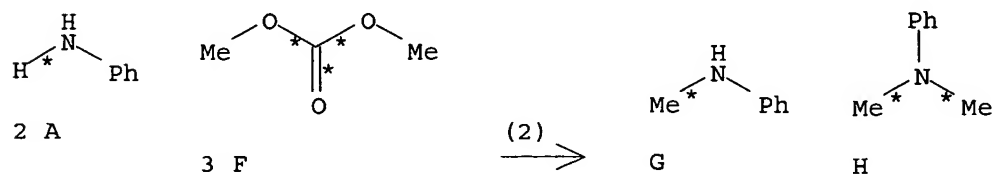
FILE 'CAPLUS' ENTERED AT 15:54:05 ON 03 MAY 2006
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 PROCESSING COMPLETED FOR L58
 PROCESSING COMPLETED FOR L59

L60 44 DUP REM L58 L59 (1 DUPLICATE REMOVED)
 ANSWERS '1-41' FROM FILE CASREACT
 ANSWERS '42-44' FROM FILE CAPLUS

=> d ibib abs hit L60 1-41; d ibib abs hitind hitstr L60 42-44

L60 ANSWER 1 OF 44 CASREACT COPYRIGHT 2006 ACS on STN DUPLICATE 1
 ACCESSION NUMBER: 141:395224 CASREACT
 TITLE: Zeolite-promoted selective mono-N-methylation of
 aniline with dimethyl carbonate
 AUTHOR(S): Esakkidurai, Thirugnanasamy; Pitchumani, Kasi
 CORPORATE SOURCE: School of Chemistry, Madurai Kamaraj University,
 Madurai, 625021, India
 SOURCE: Journal of Molecular Catalysis A: Chemical (2004),
 218(2), 197-201
 CODEN: JMCCF2; ISSN: 1381-1169
 PUBLISHER: Elsevier Science B.V.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Selective mono-N-methylation of aniline with di-Me carbonate is carried
 out over **faujasite** Y zeolites. This one pot protocol is highly
 selective, favoring mono-N-methylation. Benzylolation with dibenzyl
 carbonate is also found to be very selective, resulting in exclusive
 monobenzylation. Other advantages such as lower temperature, less rigorous
 reaction conditions, absence of C-alkylation products, etc., are also
 highlighted.

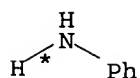
RX(2) OF 9 2 A + 3 F ==> G + H



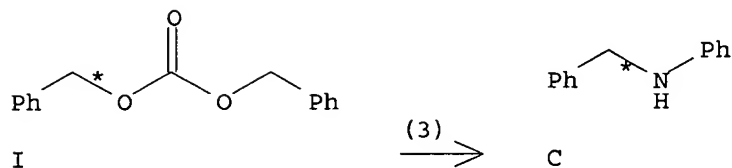
RX(2) RCT A 62-53-3, F 616-38-6
 PRO G 100-61-8, H 121-69-7

SOL 71-43-2 Benzene
 CON 205 minutes, 100 deg C
 NTE 98% conversion observed, 99:1 mono:di, Zeolite KY used as catalyst, conversion and mono-/di-selectivity depend on zeolite and reaction time, green chem.-catalyst, green chem.-waste redn., no reaction observed in the absence of zeolite

RX(3) OF 9 A + I ==> C

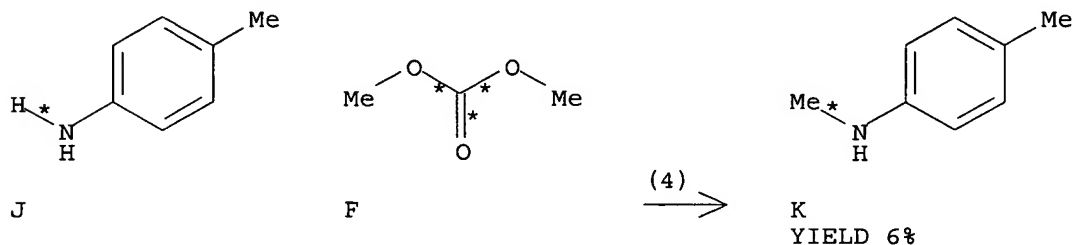


A



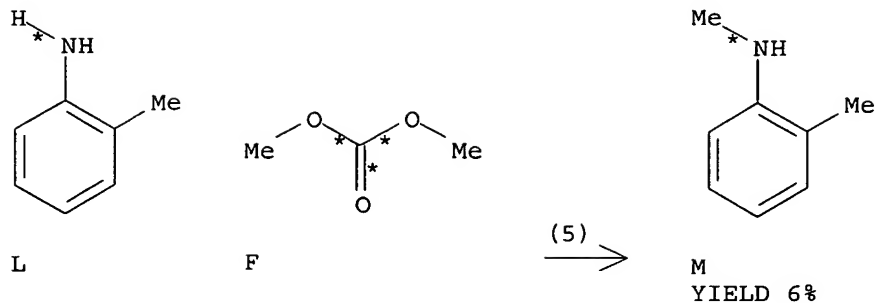
RX(3) RCT A 62-53-3, I 3459-92-5
 PRO C 103-32-2
 SOL 71-43-2 Benzene
 CON 100 deg C
 NTE 100:0 mono:di, 77% conversion observed, Zeolite NaX used as catalyst, conversion depends on zeolite and solvent, green chem.-catalyst, green chem.-waste redn.

RX(4) OF 9 J + F ==> K



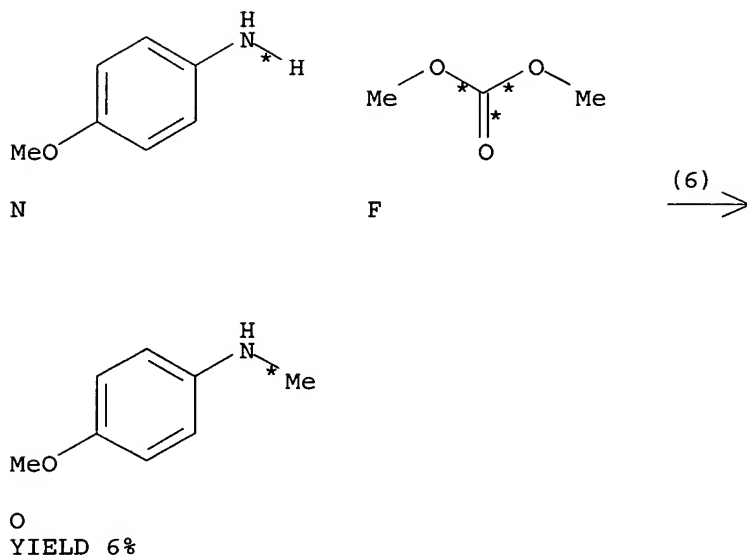
RX(4) RCT J 106-49-0, F 616-38-6
 PRO K 623-08-5
 SOL 71-43-2 Benzene
 CON 205 minutes, 100 deg C
 NTE Zeolite KY used as catalyst, green chem.-catalyst, green chem.-waste redn.

RX(5) OF 9 L + F ==> M



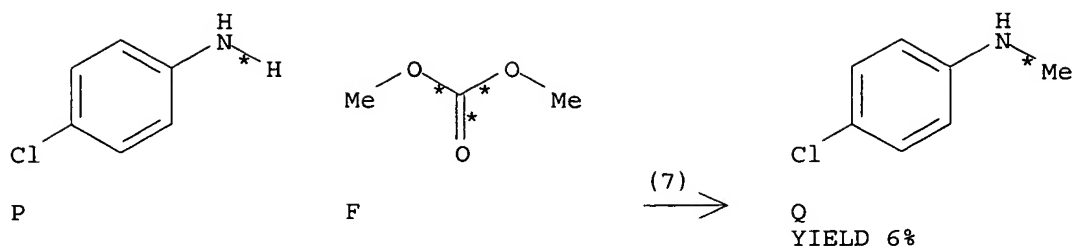
RX(5) RCT L 95-53-4, F 616-38-6
 PRO M 611-21-2
 SOL 71-43-2 Benzene
 CON 205 minutes, 100 deg C
 NTE Zeolite KY used as catalyst, green chem.-catalyst, green chem.-waste redn.

RX(6) OF 9 N + F ==> O



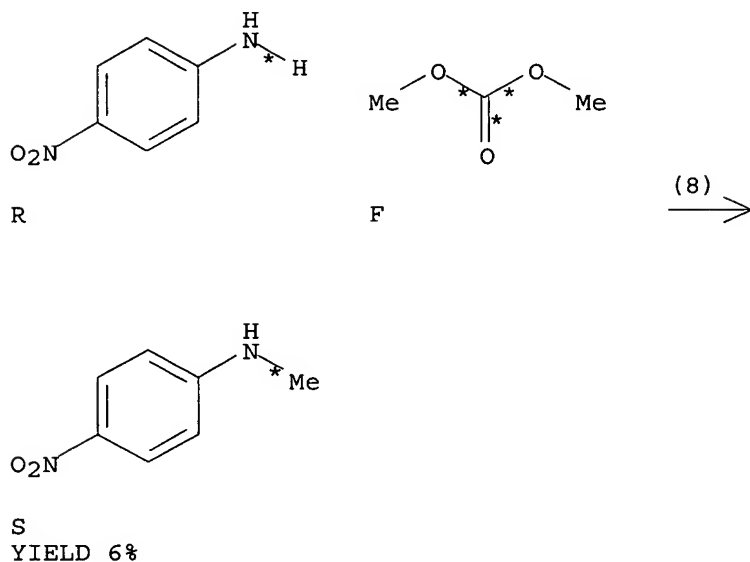
RX(6) RCT N 104-94-9, F 616-38-6
 PRO O 5961-59-1
 SOL 71-43-2 Benzene
 CON 205 minutes, 100 deg C
 NTE Zeolite KY used as catalyst, green chem.-catalyst, green chem.-waste redn.

RX(7) OF 9 P + F ==> Q



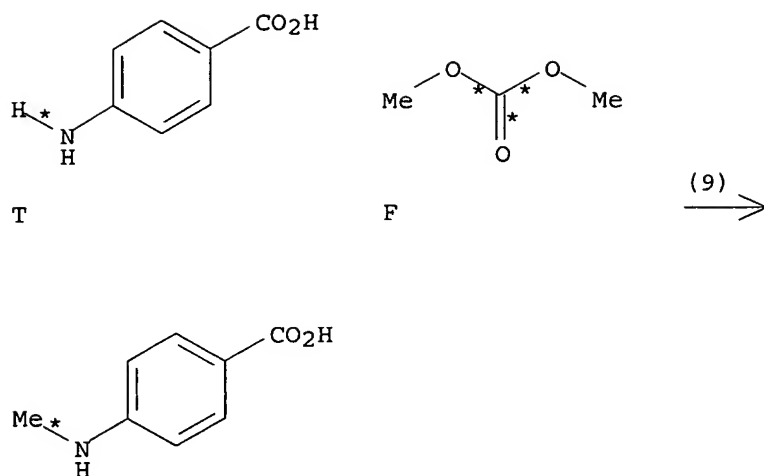
RX(7) RCT P 106-47-8, F 616-38-6
 PRO Q 932-96-7
 SOL 71-43-2 Benzene
 CON 205 minutes, 100 deg C
 NTE Zeolite KY used as catalyst, green chem.-catalyst, green
 chem.-waste redn.

RX(8) OF 9 R + F ==> S



RX(8) RCT R 100-01-6, F 616-38-6
 PRO S 100-15-2
 SOL 71-43-2 Benzene
 CON 205 minutes, 100 deg C
 NTE Zeolite KY used as catalyst, green chem.-catalyst, green
 chem.-waste redn.

RX(9) OF 9 T + F ==> U



U
YIELD 6%

RX(9) RCT T 150-13-0, F 616-38-6
 PRO U 10541-83-0
 SOL 71-43-2 Benzene
 CON 205 minutes, 100 deg C
 NTE Zeolite KY used as catalyst, green chem.-catalyst, green chem.-waste redn.

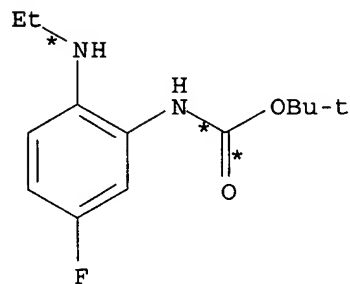
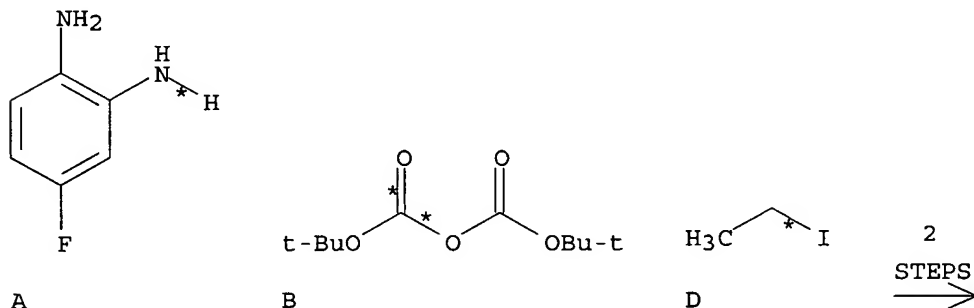
AB Selective mono-N-methylation of aniline with di-Me carbonate is carried out over **faujasite Y** zeolites. This one pot protocol is highly selective, favoring mono-N-methylation. Benzoylation with dibenzyl carbonate is also found to be very selective, resulting in exclusive monobenzoylation. Other advantages such as lower temperature, less rigorous reaction conditions, absence of C-alkylation products, etc., are also highlighted.

ST aniline selective methylation benzoylation; **faujasite Y** zeolite selective methylation benzoylation catalyst; methylaniline benzylaniline prepn

160 ANSWER 2 OF 44 CASREACT COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 143:229795 CASREACT
 TITLE: (1H-Imidazo[4,5-c]pyridin-2-yl)-1,2,5-oxadiazol-3-ylamine derivatives: A novel class of potent MSK-1-inhibitors
 AUTHOR(S): Bamford, Mark J.; Alberti, Michael J.; Bailey, Nicholas; Davies, Susannah; Dean, David K.; Gaiba, Alessandra; Garland, Stephen; Harling, John D.; Jung, David K.; Panchal, Terence A.; Parr, Christopher A.; Steadman, Jon G.; Takle, Andrew K.; Townsend, James T.; Wilson, David M.; Witherington, Jason
 CORPORATE SOURCE: Neurology and GI Centre of Excellence for Drug Discovery, New Frontiers Science Park, GlaxoSmithKline Pharmaceuticals, Essex, CM19 5AW, UK
 SOURCE: Bioorganic & Medicinal Chemistry Letters (2005), 15(14), 3402-3406
 CODEN: BMCLE8; ISSN: 0960-894X
 PUBLISHER: Elsevier B.V.

DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB A novel series of imidazo[4,5-c]pyridines bearing a 1,2,5-oxadiazol-3-ylamine functionality has been developed. These are potent inhibitors of mitogen and stress-activated protein kinase-1.
 REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(28) OF 60 COMPOSED OF RX(1), RX(2)
 RX(28) A + B + D ==> E



E
 YIELD 38%

RX(1) RCT A 367-31-7, B 24424-99-5
 PRO C 362670-07-3
 CON 50 deg C
 NTE regioselective

RX(2) RCT C 362670-07-3

STAGE(1)

RGT F 865-47-4 t-BuOK
 SOL 109-99-9 THF
 CON 21 deg C

STAGE(2)

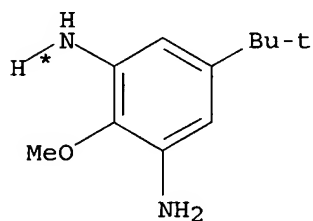
RCT D 75-03-6
 CON 21 deg C

PRO E 862815-01-8

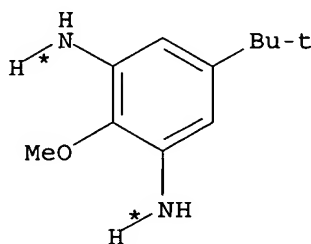
✓

L60 ANSWER 3 OF 44 CASREACT COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 143:59953 CASREACT
 TITLE: Exhaustively Methylated Azacalix[4]arene: Preparation, Conformation, and Crystal Structure with Exclusively CH/ π -Controlled Crystal Architecture
 AUTHOR(S): Tsue, Hirohito; Ishibashi, Koichi; Takahashi, Hiroki; Tamura, Rui
 CORPORATE SOURCE: Graduate School of Global Environmental Studies and Graduate School of Human and Environmental Studies, Kyoto University, Kyoto, 606-8501, Japan
 SOURCE: Organic Letters (2005), 7(11), 2165-2168
 CODEN: ORLEF7; ISSN: 1523-7060
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB The preparation, conformation, and crystal structure of exhaustively methylated azacalix[4]arene involving nitrogen atoms as bridging units are described. NMR and X-ray crystallog. anal. have demonstrated that this novel azacalix[4]arene adopts a 1,3-alternate conformation both in solution and in the solid state. The crystal structure has been characterized solely by intermol. CH/ π interactions, by which the azacalix[4]arenes mutually interact with each other outside the cavity to furnish a two-dimensional network structure.
 REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

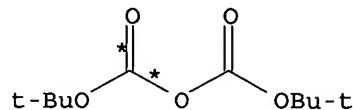
RX(9) OF 19 COMPOSED OF RX(2), RX(3)
 RX(9) 2 B + 2 H + 2 L ==> M



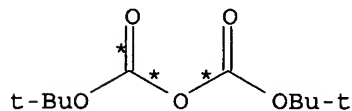
B



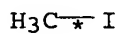
B



H

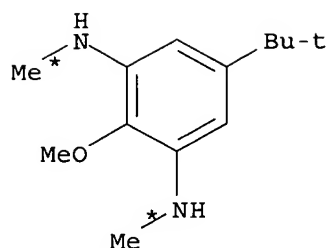


H



2 L

2
 STEPS
 →



M
YIELD 72%

RX (2) RCT B 473269-70-4, H 24424-99-5
PRO I 854669-26-4, J 854669-30-0
SOL 75-65-0 t-BuOH
CON 3 hours, room temperature

RX (3) RCT J 854669-30-0

STAGE (1)

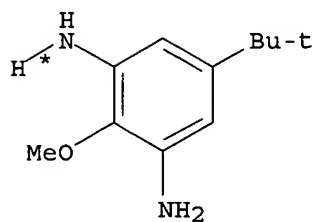
RGT N 7646-69-7 NaH
SOL 68-12-2 DMF
CON 10 minutes, 0 deg C

STAGE (2)

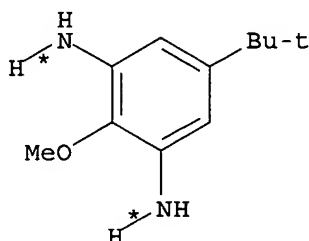
RCT L 74-88-4
CON SUBSTAGE (1) 0 deg C
SUBSTAGE (2) overnight, room temperature

PRO M 854669-37-7

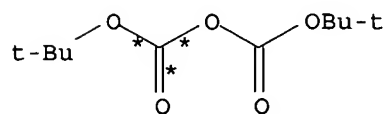
RX (14) OF 19 COMPOSED OF RX (2), RX (4), RX (5)
RX (14) 2 B + 2 H + C + 3 L ==> Q



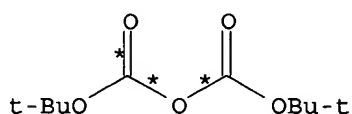
B



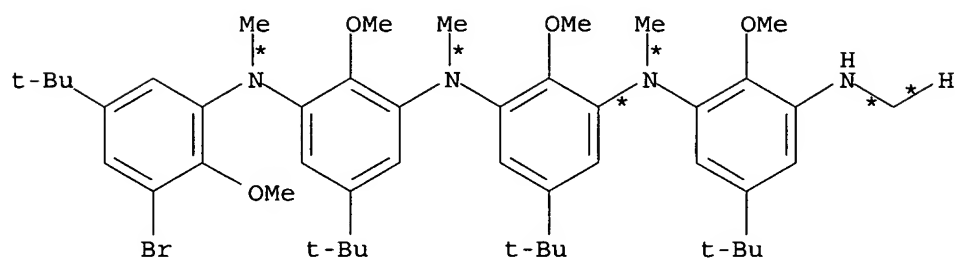
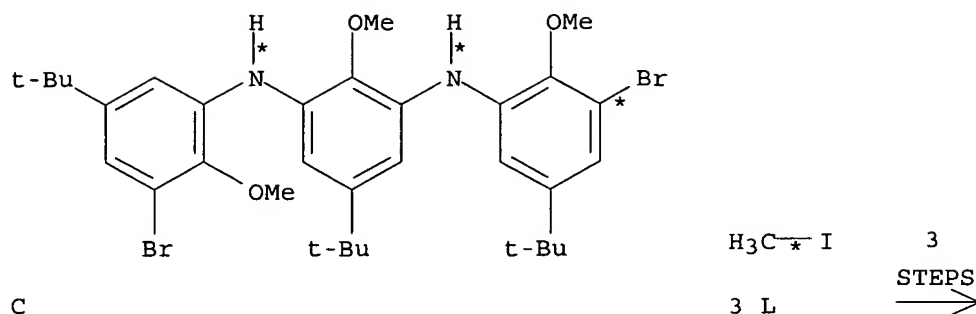
B



H



H



RX(2) RCT B 473269-70-4, H 24424-99-5
 PRO I 854669-26-4, J 854669-30-0
 SOL 75-65-0 t-BuOH
 CON 3 hours, room temperature

RX(4) RCT C 854669-22-0, I 854669-26-4
 RGT D 865-48-5 NaOBu-t
 PRO P 854669-43-5
 CAT 166330-10-5 Phosphine, (oxydi-2,1-phenylene)bis[diphenyl-,
 3375-31-3 Pd(OAc)₂
 SOL 108-88-3 PhMe
 CON 22 hours, 80 deg C

RX(5) RCT P 854669-43-5

STAGE(1)

RGT N 7646-69-7 NaH
 SOL 68-12-2 DMF
 CON 10 minutes, 0 deg C

STAGE(2)

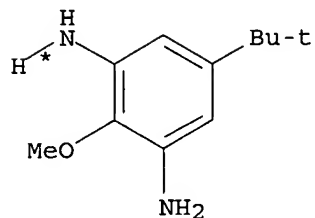
RCT L 74-88-4
 CON SUBSTAGE(1) 0 deg C
 SUBSTAGE(2) overnight, room temperature

PRO Q 854669-49-1

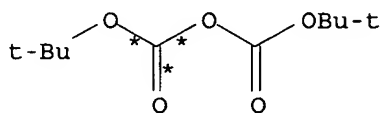
RX(18) OF 19 COMPOSED OF REACTION SEQUENCE RX(2), RX(4), RX(5)
AND REACTION SEQUENCE RX(1), RX(4), RX(5)

...2 B + 2 H ==> I...

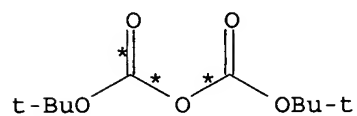
...2 A + B + I + 3 L ==> Q



B

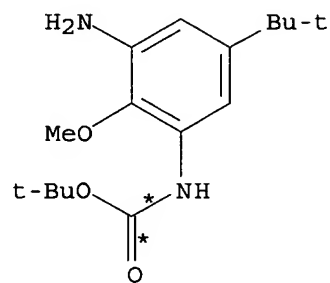


H



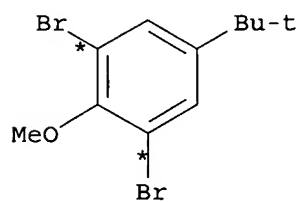
H

3
STEPS
→

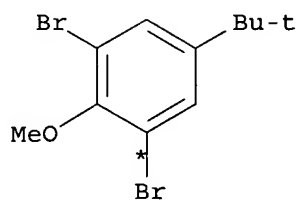


I

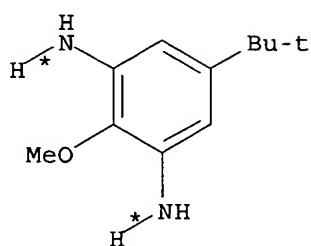
START NEXT REACTION SEQUENCE



A



A



2 B

STAGE(2)

RCT L 74-88-4

CON SUBSTAGE(1) 0 deg C

SUBSTAGE(2) overnight, room temperature

PRO Q 854669-49-1

✓ L60 ANSWER 4 OF 44 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 142:411301 CASREACT

TITLE: Inhibition of secretory phospholipase A2. 2-Synthesis and structure-activity relationship studies of 4,5-dihydro-3-(4-tetradecyloxybenzyl)-1,2,4-4H-oxadiazol-5-one (PMS1062) derivatives specific for group II enzyme

AUTHOR(S): Dong, Chang-Zhi; Ahamada-Himidi, Azali; Plocki, Stephanie; Aoun, Darina; Touaibia, Mohamed; Meddad-Bel Habich, Nadia; Huet, Jack; Redeuilh, Catherine; Ombetta, Jean-Edouard; Godfroid, Jean-Jacques; Massicot, France; Heymans, Francoise

CORPORATE SOURCE: Unite de Pharmacochimie Moleculaire et Systemes Membranaires (EA2381), Laboratoire de Pharmacochimie Moleculaire, Universite Paris 7-Denis Diderot, Paris, 75251, Fr.

SOURCE: Bioorganic & Medicinal Chemistry (2005), 13(6), 1989-2007

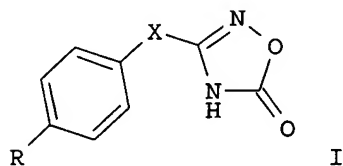
CODEN: BMECEP; ISSN: 0968-0896

PUBLISHER: Elsevier Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

GI

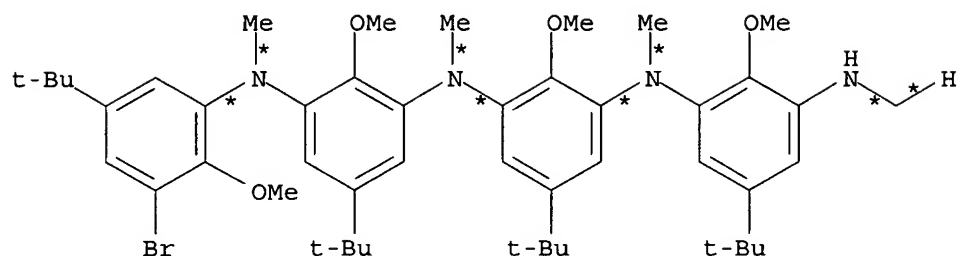
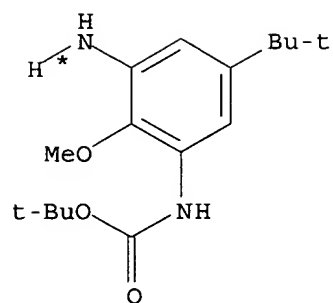


AB The discovery of a series of specific inhibitors of human group IIA phospholipase A2 (hGIIA PLA2) displaying promising in vitro and in vivo properties has been recently reported. Here the influence of different structural modifications on the specificity and potency of oxadiazolones, e.g. I [X = CH₂, CH₂CH₂, CHMe, CMe₂; R = MeO, n-octyloxy, n-tetradecylthio, N,N-di(heptyl)amino, etc.], against hGIIA PLA2 vs. porcine group IB PLA2 is described. The SAR results, as well as the log P and pK_a values of the oxadiazolones studied provide important information towards the comprehension of the mode of action of this kind of compds.

REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(226) OF 226 COMPOSED OF RX(29), RX(30), RX(50), RX(74), RX(75)

RX(226) 3 W + 2 BW + CB + DD ==> ED



Q
YIELD 81%

RX (2) RCT B 473269-70-4, H 24424-99-5
PRO I 854669-26-4, J 854669-30-0
SOL 75-65-0 t-BuOH
CON 3 hours, room temperature

RX (1) RCT A 132268-08-7, B 473269-70-4
RGT D 865-48-5 NaOBu-t
PRO C 854669-22-0
CAT 166330-10-5 Phosphine, (oxydi-2,1-phenylene)bis[diphenyl-,
3375-31-3 Pd(OAc)₂
SOL 108-88-3 PhMe
CON 24 hours, 80 deg C

RX (4) RCT C 854669-22-0, I 854669-26-4
RGT D 865-48-5 NaOBu-t
PRO P 854669-43-5
CAT 166330-10-5 Phosphine, (oxydi-2,1-phenylene)bis[diphenyl-,
3375-31-3 Pd(OAc)₂
SOL 108-88-3 PhMe
CON 22 hours, 80 deg C

RX (5) RCT P 854669-43-5

STAGE (1)
RGT N 7646-69-7 NaH
SOL 68-12-2 DMF
CON 10 minutes, 0 deg C

STAGE(2)

SOL 108-88-3 PhMe
CON 5 hours, reflux

PRO EC 850143-73-6

RX(75) RCT EC 850143-73-6
RGT U 7647-01-0 HCl
PRO ED 850143-74-7
SOL 60-29-7 Et2O, 109-99-9 THF
CON SUBSTAGE(1) 2 hours, 0 deg C
SUBSTAGE(2) 1 hour, room temperature

L60 ANSWER 5 OF 44 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 142:316675 CASREACT

TITLE: Optimization of 6,7-Disubstituted-4-(arylamino)quinoline-3-carbonitriles as Orally Active, Irreversible Inhibitors of Human Epidermal Growth Factor Receptor-2 Kinase Activity

AUTHOR(S): Tsou, Hwei-Ru; Overbeek-Klumpers, Elsebe G.; Hallett, William A.; Reich, Marvin F.; Floyd, M. Brawner; Johnson, Bernard D.; Michalak, Ronald S.; Nilakantan, Ramaswamy; Discafani, Carolyn; Golas, Jonathan; Rabindran, Sridhar K.; Shen, Ru; Shi, Xiaoqing; Wang, Yu-Fen; Upeslakis, Janis; Wissner, Allan

CORPORATE SOURCE: Chemical and Screening Sciences, Chemical Development, and Oncology, Wyeth Research, Pearl River, NY, 10965, USA

SOURCE: Journal of Medicinal Chemistry (2005), 48(4), 1107-1131

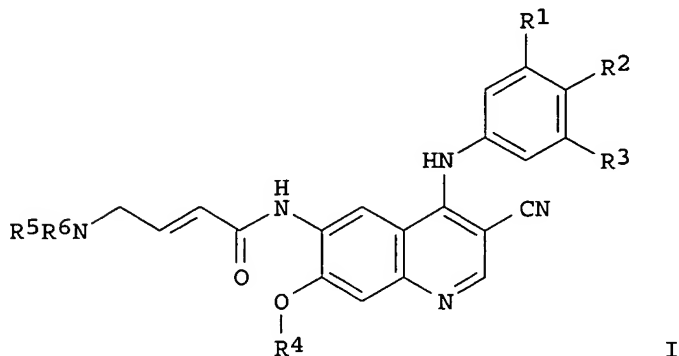
CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

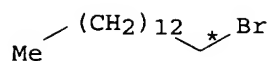
DOCUMENT TYPE: Journal

LANGUAGE: English

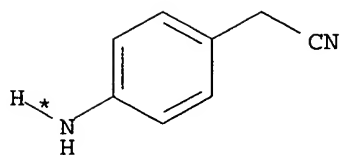
GI



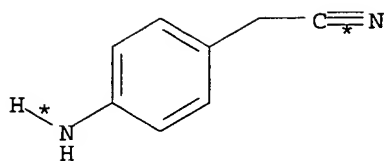
AB A series of new 6,7-disubstituted-4-(arylamino)quinoline-3-carbonitriles, e.g. I (R1 = H, Cl; R2 = PhCH2O, 1-imidazolyl, 2-furylmethoxy, etc.; R3 = Cl, CN, PhCH2O; R4 = Me, Et; R5 = Me, R6 = Me, HOCH2CH2; R5R6N = azetidiny, piperidiny, thiomorpholinyl, etc.) that function as irreversible inhibitors of human epidermal growth factor receptor-2



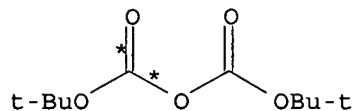
3 W



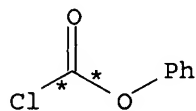
BW



BW

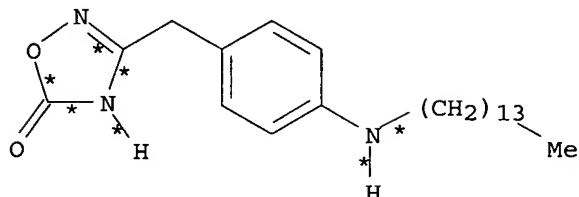


CB



DD

5
STEPS
→



ED

YIELD 44%

RX(29) RCT W 112-71-0, BW 3544-25-0
 RGT BL 584-08-7 K₂CO₃
 PRO BZ 850143-36-1, CA 850143-37-2
 SOL 75-05-8 MeCN
 CON 1 month, reflux

RX(30) RCT CA 850143-37-2, CB 24424-99-5
 RGT BL 584-08-7 K₂CO₃
 PRO CC 850143-38-3
 SOL 75-05-8 MeCN, 123-91-1 Dioxane
 CON SUBSTAGE(1) 7 days, room temperature
 SUBSTAGE(2) 14 days, reflux

RX(50) RCT CC 850143-38-3
 RGT CF 5470-11-1 H₂NOH-HCl, BL 584-08-7 K₂CO₃
 PRO CY 850143-55-4
 SOL 64-17-5 EtOH
 CON 18 hours, reflux

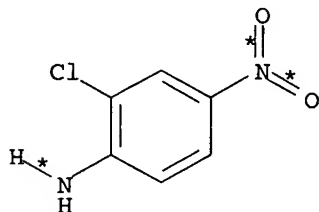
RX(74) RCT CY 850143-55-4, DD 1885-14-9

STAGE(1)
 RGT E 121-44-8 Et₃N
 SOL 67-66-3 CHCl₃
 CON 1 hour, 0 deg C

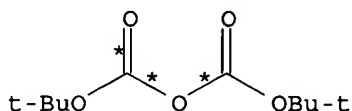
(HER-2) and epidermal growth factor receptor (EGFR) kinases have been prepared. These compounds demonstrated enhanced activities for inhibiting HER-2 kinase and the growth of HER-2 pos. cells compared to the EGFR kinase inhibitor I [R1 = H; R2 = F; R3 = Cl; R4 = Et; R5 = R6 = Me; (EKB-569)]. Three synthetic routes were used to prepare these compounds. They were prepared mostly by acylation of 6-amino-4-(arylamino)quinoline-3-carbonitriles with unsatd. acid chlorides or by amination of 4-chloro-6-(crotonamido)quinoline-3-carbonitriles with monocyclic or bicyclic anilines. The third route was developed to prepare a key intermediate, 6-acetamido-4-chloroquinoline-3-carbonitrile, that involved a safer cyclization step. It was shown that attaching a large lipophilic group at the para position of the 4-(arylamino) ring results in improved potency for inhibiting HER-2 kinase. The importance of a basic dialkylamino group at the end of the Michael acceptor for activity, due to intramol. catalysis of the Michael addition has also been demonstrated. This, along with improved water solubility, resulted in compounds with enhanced biol. properties. The mol. modeling results consistent with the proposed mechanism of inhibition are presented. Binding studies of one compound, I [R1 = H; R2 = 2-pyridylmethoxy; R3 = Cl; R4 = Et; R5 = R6 = Me; (HKI-272)] (C-14 radiolabeled), showed that it binds irreversibly to HER-2 protein in BT474 cells. Furthermore, it demonstrated excellent oral activity, especially in HER-2 overexpressing xenografts. Compound HKI-272 was selected for further studies and is currently in phase I clin. trials for the treatment of cancer.

REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

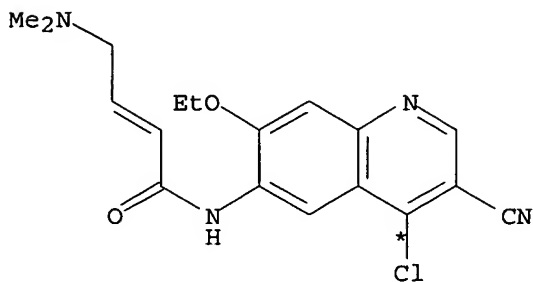
RX(290) OF 368 COMPOSED OF RX(109), RX(110), RX(111), RX(112)
 RX(290) IK + IL + GO + IR ==> IS



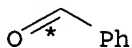
IK



IL

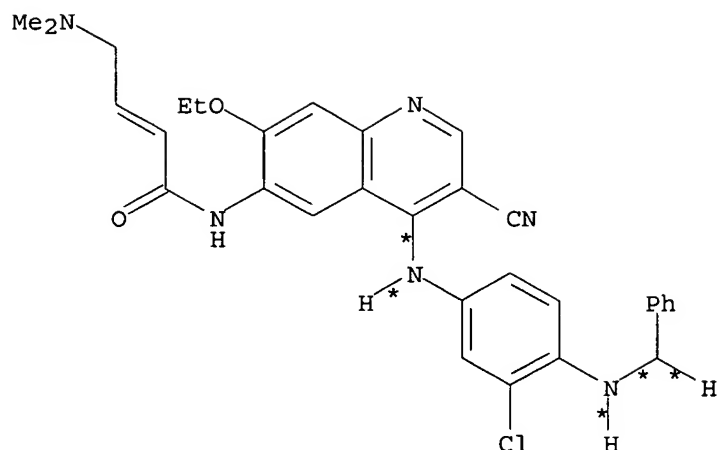


GO



IR

4
 STEPS
 →



IS
YIELD 68%

```

RX(109)  RCT  IK 121-87-9, IL 24424-99-5
          PRO  IM 252019-65-1
          CAT  1122-58-3 4-DMAP
          SOL  109-99-9 THF
          CON  SUBSTAGE(1) 0 deg C
                SUBSTAGE(2) 0 deg C -> 25 deg C
                SUBSTAGE(3) 3 hours, 25 deg C

RX(110)  RCT  IM 252019-65-1
          RGT  G 7439-89-6 Fe
          PRO  IO 252019-51-5
          SOL  67-56-1 MeOH, 64-19-7 AcOH
          CON  30 minutes, reflux

RX(111)  RCT  GO 848133-88-0, IO 252019-51-5

          STAGE(1)
            RGT  BO 628-13-7 Pyridinium chloride
            SOL  109-86-4 MeCH2CH2OH
            CON  1 hour, reflux

          STAGE(2)
            RGT  AK 584-08-7 K2CO3
            SOL  7732-18-5 Water
            CON  room temperature, pH 9

          STAGE(3)
            RGT  IQ 76-05-1 F3CCO2H
            SOL  75-09-2 CH2Cl2
            CON  SUBSTAGE(1) 0 deg C
                  SUBSTAGE(2) 0 deg C -> 25 deg C
                  SUBSTAGE(3) 15 minutes, 25 deg C

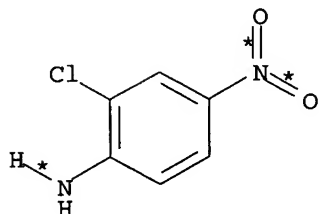
          PRO  IP 848134-31-6

RX(112)  RCT  IP 848134-31-6, IR 100-52-7
          RGT  IT 56553-60-7 Na.(AcO)3BH, I 64-19-7 AcOH

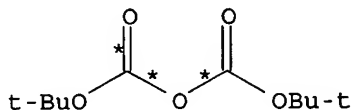
```

PRO IS 848134-32-7
 SOL 107-06-2 ClCH₂CH₂Cl
 CON 18 hours, 25 deg C

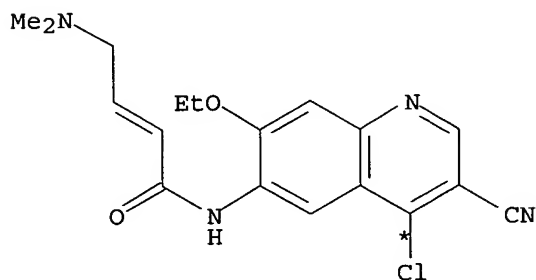
RX(291) OF 368 COMPOSED OF RX(109), RX(110), RX(111), RX(113)
 RX(291) IK + IL + GO + IV ==> IW



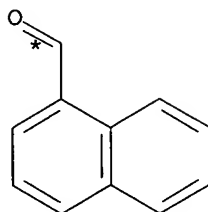
IK



IL



GO



IV

4
 STEPS
 →

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RX(109) RCT IK 121-87-9, IL 24424-99-5
 PRO IM 252019-65-1
 CAT 1122-58-3 4-DMAP
 SOL 109-99-9 THF
 CON SUBSTAGE(1) 0 deg C
 SUBSTAGE(2) 0 deg C -> 25 deg C
 SUBSTAGE(3) 3 hours, 25 deg C

RX(110) RCT IM 252019-65-1
 RGT G 7439-89-6 Fe
 PRO IO 252019-51-5
 SOL 67-56-1 MeOH, 64-19-7 AcOH
 CON 30 minutes, reflux

RX(111) RCT GO 848133-88-0, IO 252019-51-5

STAGE(1)
 RGT BO 628-13-7 Pyridinium chloride
 SOL 109-86-4 MeCH₂CH₂OH
 CON 1 hour, reflux

STAGE(2)

RGT AK 584-08-7 K₂CO₃
 SOL 7732-18-5 Water
 CON room temperature, pH 9

STAGE(3)

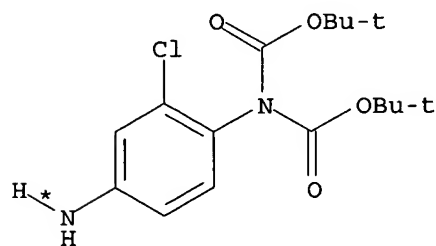
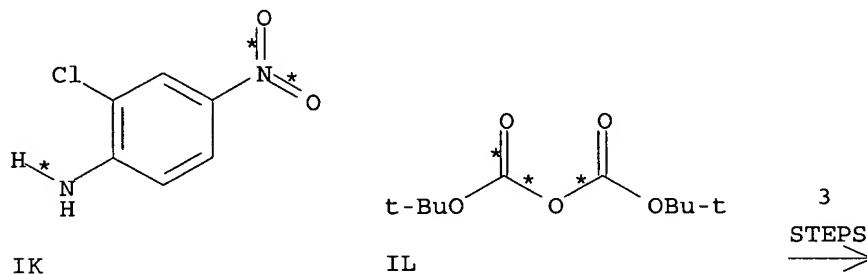
RGT IQ 76-05-1 F₃CCO₂H
 SOL 75-09-2 CH₂Cl₂
 CON SUBSTAGE(1) 0 deg C
 SUBSTAGE(2) 0 deg C -> 25 deg C
 SUBSTAGE(3) 15 minutes, 25 deg C

PRO IP 848134-31-6

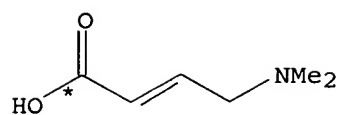
RX(113) RCT IP 848134-31-6, IV 66-77-3
 RGT IT 56553-60-7 Na.(AcO)₃BH, I 64-19-7 AcOH
 PRO IW **848134-33-8**
 SOL 107-06-2 ClCH₂CH₂Cl
 CON 18 hours, 25 deg C

RX(348) OF 368 COMPOSED OF REACTION SEQUENCE RX(109), RX(110), RX(111), RX(112)
 AND REACTION SEQUENCE RX(85), RX(111), RX(112)

...IK + IL ==> IO...
 ...DQ + GN + IO + IR ==> IS

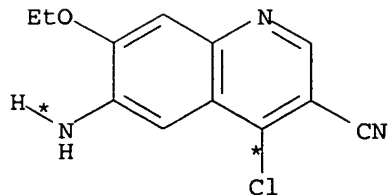


START NEXT REACTION SEQUENCE

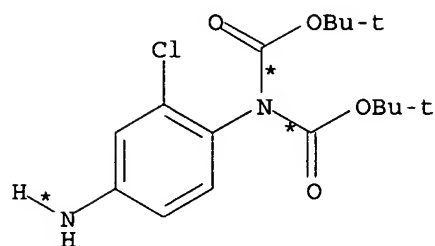


● HCl

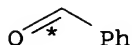
DQ



GN

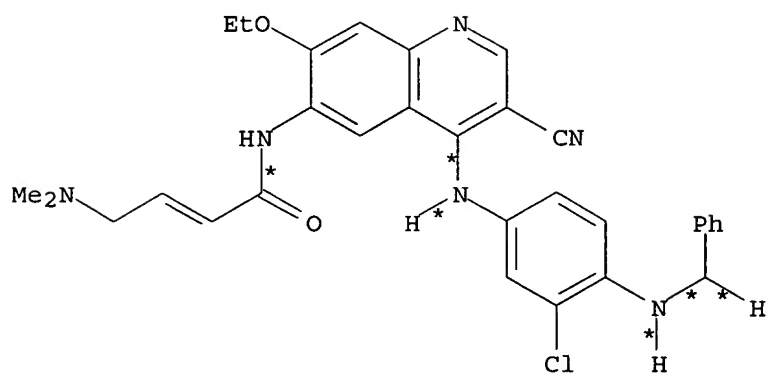


IO



IR

3
STEPS
→



IS

YIELD 68%

RX(109) RCT IK 121-87-9, IL 24424-99-5
 PRO IM 252019-65-1
 CAT 1122-58-3 4-DMAP
 SOL 109-99-9 THF
 CON SUBSTAGE(1) 0 deg C
 SUBSTAGE(2) 0 deg C -> 25 deg C
 SUBSTAGE(3) 3 hours, 25 deg C

RX(110) RCT IM 252019-65-1
 RGT G 7439-89-6 Fe
 PRO IO 252019-51-5

SOL 67-56-1 MeOH, 64-19-7 AcOH
CON 30 minutes, reflux

RX(85) RCT DQ 848133-35-7

STAGE(1)
RGT DT 79-37-8 (COCl)₂
CAT 68-12-2 DMF
SOL 75-05-8 MeCN
CON 30 minutes, 60 deg C

STAGE(2)
RCT GN 848133-87-9
SOL 872-50-4 NMEP
CON 2.5 hours, 0 deg C

PRO GO 848133-88-0

RX(111) RCT GO 848133-88-0, IO 252019-51-5

STAGE(1)
RGT BO 628-13-7 Pyridinium chloride
SOL 109-86-4 MeCH₂CH₂OH
CON 1 hour, reflux

STAGE(2)
RGT AK 584-08-7 K₂CO₃
SOL 7732-18-5 Water
CON room temperature, pH 9

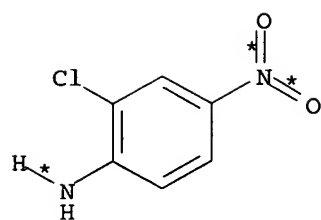
STAGE(3)
RGT IQ 76-05-1 F₃CCO₂H
SOL 75-09-2 CH₂Cl₂
CON SUBSTAGE(1) 0 deg C
SUBSTAGE(2) 0 deg C -> 25 deg C
SUBSTAGE(3) 15 minutes, 25 deg C

PRO IP 848134-31-6

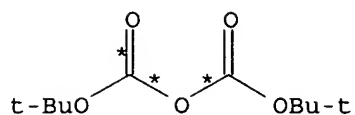
RX(112) RCT IP 848134-31-6, IR 100-52-7
RGT IT 56553-60-7 Na.(AcO)₃BH, I 64-19-7 AcOH
PRO IS **848134-32-7**
SOL 107-06-2 ClCH₂CH₂Cl
CON 18 hours, 25 deg C

RX(349) OF 368 COMPOSED OF REACTION SEQUENCE RX(109), RX(110), RX(111), RX(113)
AND REACTION SEQUENCE RX(85), RX(111), RX(113)

...IK + **IL** ==> IO...
...DQ + GN + **IO** + IV ==> **IW**

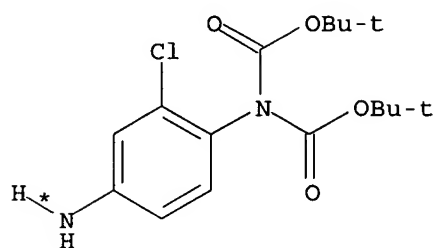


IK



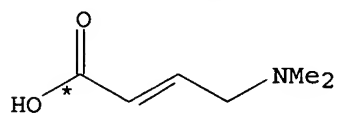
IL

3
STEPS
→



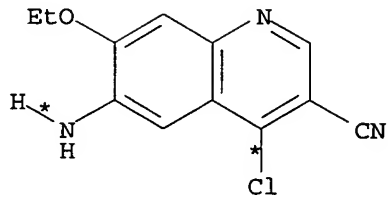
IO

START NEXT REACTION SEQUENCE

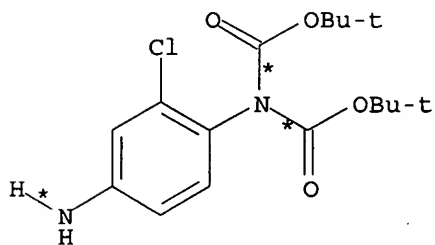


DQ

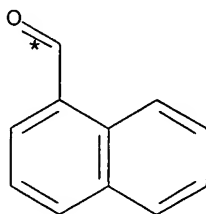
● HCl



GN

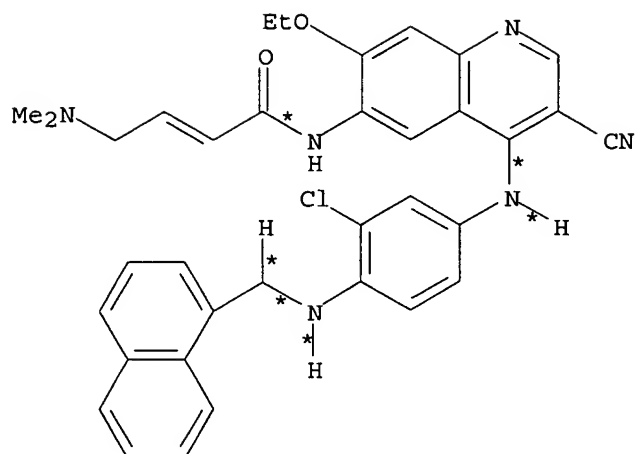


IO



IV

3
STEPS
→



IW
YIELD 91%

RX(109) RCT IK 121-87-9, IL **24424-99-5**
 PRO IM 252019-65-1
 CAT 1122-58-3 4-DMAP
 SOL 109-99-9 THF
 CON SUBSTAGE(1) 0 deg C
 SUBSTAGE(2) 0 deg C -> 25 deg C
 SUBSTAGE(3) 3 hours, 25 deg C

RX(110) RCT IM 252019-65-1
 RGT G 7439-89-6 Fe
 PRO IO 252019-51-5
 SOL 67-56-1 MeOH, 64-19-7 AcOH
 CON 30 minutes, reflux

RX(85) RCT DQ 848133-35-7
 STAGE(1)
 RGT DT 79-37-8 (COCl)₂
 CAT 68-12-2 DMF
 SOL 75-05-8 MeCN
 CON 30 minutes, 60 deg C

STAGE(2)
 RCT GN 848133-87-9
 SOL 872-50-4 NMEP
 CON 2.5 hours, 0 deg C

PRO GO 848133-88-0

RX(111) RCT GO 848133-88-0, IO **252019-51-5**

STAGE(1)
 RGT BO 628-13-7 Pyridinium chloride
 SOL 109-86-4 MeCH₂CH₂OH
 CON 1 hour, reflux

STAGE(2)

RGT AK 584-08-7 K2CO3
 SOL 7732-18-5 Water
 CON room temperature, pH 9

STAGE(3)

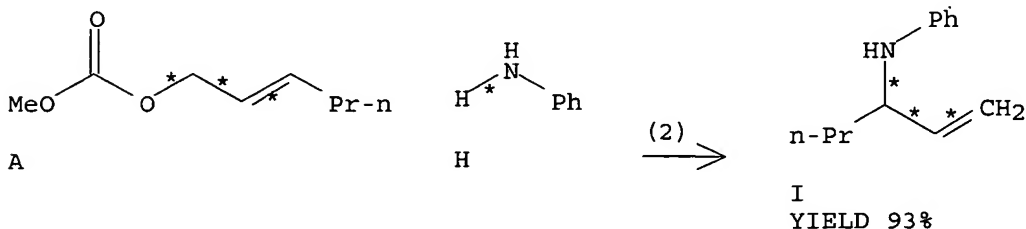
RGT IQ 76-05-1 F3CCO2H
 SOL 75-09-2 CH2Cl2
 CON SUBSTAGE(1) 0 deg C
 SUBSTAGE(2) 0 deg C -> 25 deg C
 SUBSTAGE(3) 15 minutes, 25 deg C

PRO IP 848134-31-6

RX(113) RCT IP 848134-31-6, IV 66-77-3
 RGT IT 56553-60-7 Na.(AcO)3BH, I 64-19-7 AcOH
 PRO IW 848134-33-8
 SOL 107-06-2 ClCH2CH2Cl
 CON 18 hours, 25 deg C

✓ L60 ANSWER 6 OF 44 CASREACT COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 142:218805 CASREACT
 TITLE: Effects of Catalyst Activation and Ligand Steric Properties on the Enantioselective Allylation of Amines and Phenoxides
 AUTHOR(S): Leitner, Andreas; Shu, Chutian; Hartwig, John F.
 CORPORATE SOURCE: Department of Chemistry, Yale University, New Haven, CT, 6520-8107, USA
 SOURCE: Organic Letters (2005), 7(6), 1093-1096
 CODEN: ORLEF7; ISSN: 1523-7060
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB The yields, enantioselectivities, and regioselectivities of the reactions of amines and phenoxides with allylic carbonates in the presence of a metallacyclic iridium catalyst were compared. These data show that both preactivation of the catalyst and the size of the ligand affect the yield, enantioselectivity, and regioselectivity. With the activated catalyst containing a bis-naphthethylamino group, the allylic amination and etherification of a broad range of allylic carbonates occurred in high yields and with high regioselectivities and enantioselectivities.
 REFERENCE COUNT: 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(2) OF 28 A + H ==> I



RX(2)

STAGE(1)

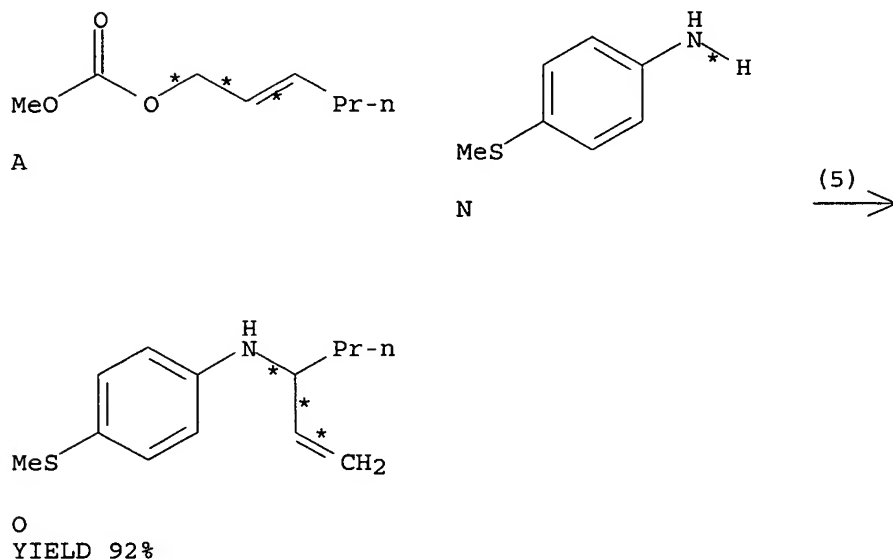
CAT 12112-67-3 Iridium, di- μ -chlorobis[(1,2,5,6- η)-1,5-cyclooctadiene]di-, 676127-12-1 Dinaphtho[2,1-d:1',2'-f][1,3,2]dioxaphosphepin-4-amine, N,N-bis[(1R)-1-(1-naphthalenyl)ethyl]-, (11bR)-, 107-10-8 PrNH₂
 SOL 109-99-9 THF
 CON 20 minutes, 50 deg C

STAGE(2)

RCT A 107574-36-7, H 62-53-3
 CON 0.5 hours, room temperature

PRO I 793726-67-7
 NTE stereoselective

RX(5) OF 28 A + N ==> O



RX(5)

STAGE(1)

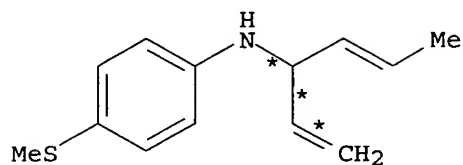
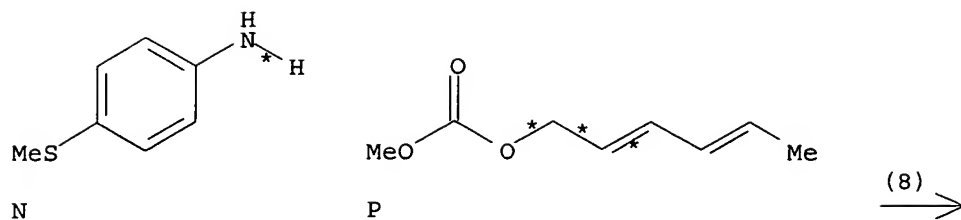
CAT 12112-67-3 Iridium, di- μ -chlorobis[(1,2,5,6- η)-1,5-cyclooctadiene]di-, 676127-12-1 Dinaphtho[2,1-d:1',2'-f][1,3,2]dioxaphosphepin-4-amine, N,N-bis[(1R)-1-(1-naphthalenyl)ethyl]-, (11bR)-, 107-10-8 PrNH₂
 SOL 109-99-9 THF
 CON 20 minutes, 50 deg C

STAGE(2)

RCT A 107574-36-7, N 104-96-1
 CON 1 hour, room temperature

PRO O 840524-20-1
 NTE stereoselective

RX(8) OF 28 N + P ==> T



T
YIELD 93%

RX(8)

STAGE(1)

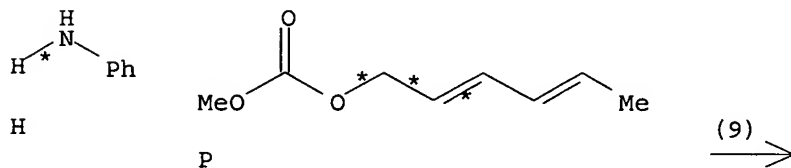
CAT 12112-67-3 Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di-, 676127-12-1 Dinaphtho[2,1-d:1',2'-f][1,3,2]dioxaphosphepin-4-amine, N,N-bis[(1R)-1-(1-naphthalenyl)ethyl]-, (11bR)-, 280-57-9 Triethylenediamine
SOL 109-99-9 THF

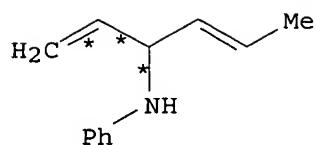
STAGE(2)

RCT N 104-96-1, P 675608-09-0
CON 2 hours, room temperature

PRO T 840524-23-4
NTE stereoselective

RX(9) OF 28 H + P ==> U





U
YIELD 81%

RX(9)

STAGE(1)

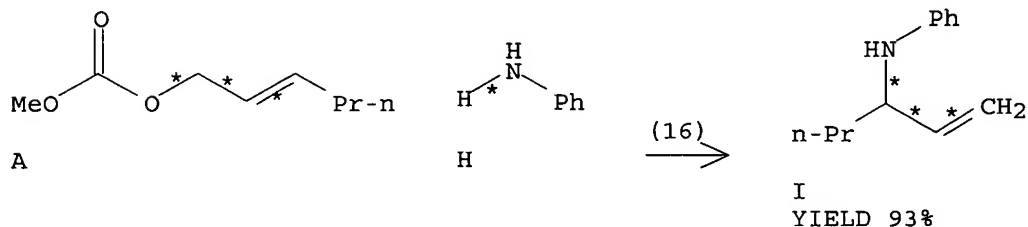
CAT 12112-67-3 Iridium, di- μ -chlorobis[(1,2,5,6- η)-1,5-cyclooctadiene]di-, 676127-12-1 Dinaphtho[2,1-d:1',2'-f][1,3,2]dioxaphosphepin-4-amine, N,N-bis[(1R)-1-(1-naphthalenyl)ethyl]-, (11bR)-, 280-57-9 Triethylenediamine
SOL 109-99-9 THF

STAGE(2)

RCT H 62-53-3, P 675608-09-0
CON 3 hours, room temperature

PRO U 840524-24-5
NTE stereoselective

RX(16) OF 28 A + H ==> I



RX(16)

STAGE(1)

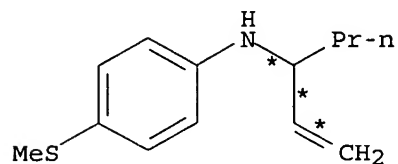
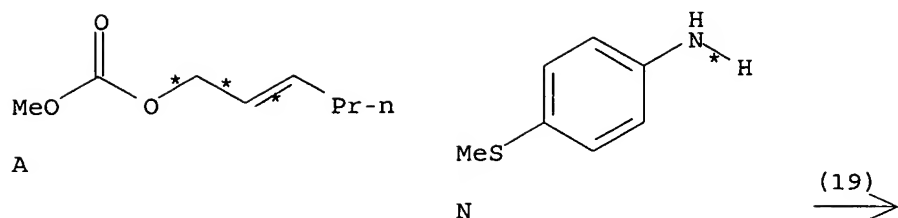
CAT 12112-67-3 Iridium, di- μ -chlorobis[(1,2,5,6- η)-1,5-cyclooctadiene]di-, 415918-91-1 Dinaphtho[2,1-d:1',2'-f][1,3,2]dioxaphosphepin-4-amine, N,N-bis[(1R)-1-phenylethyl]-, (11bR)-, 107-10-8 PrNH2
SOL 109-99-9 THF

STAGE(2)

RCT A 107574-36-7, H 62-53-3
CON 3 hours, room temperature

PRO I 793726-67-7
NTE stereoselective

RX(19) OF 28 A + N ==> O



O
YIELD 94%

RX(19)

STAGE(1)

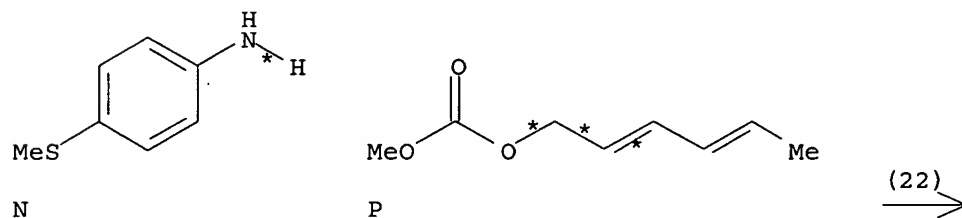
CAT 12112-67-3 Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di-, 415918-91-1 Dinaphtho[2,1-d:1',2'-f][1,3,2]dioxaphosphepin-4-amine, N,N-bis[(1R)-1-phenylethyl]-, (11bR)-, 107-10-8 PrNH₂
SOL 109-99-9 THF

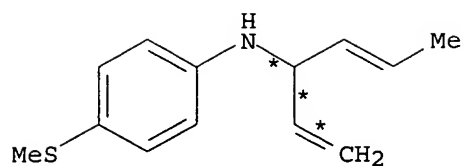
STAGE(2)

RCT A 107574-36-7, N 104-96-1
CON 3 hours, room temperature

PRO O 840524-20-1
NTE stereoselective

RX(22) OF 28 N + P ==> T





T
YIELD 73%

RX(22)

STAGE(1)

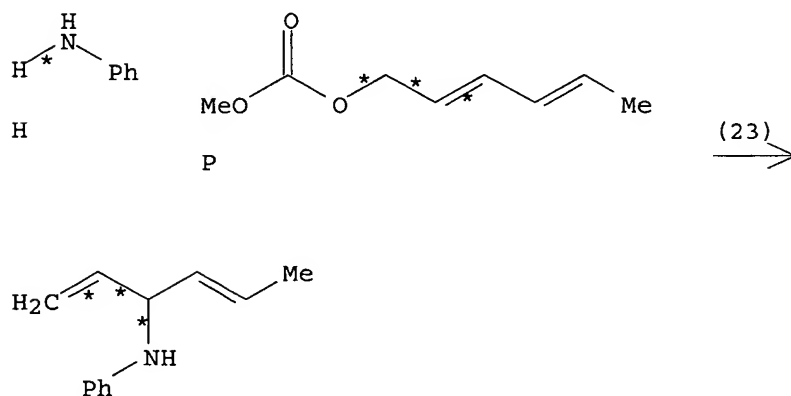
CAT 12112-67-3 Iridium, di- μ -chlorobis[(1,2,5,6- η)-1,5-cyclooctadiene]di-, 415918-91-1 Dinaphtho[2,1-d:1',2'-f][1,3,2]dioxaphosphepin-4-amine, N,N-bis[(1R)-1-phenylethyl]-, (11bR)-, 280-57-9 Triethylenediamine
SOL 109-99-9 THF

STAGE(2)

RCT N 104-96-1, P 675608-09-0
CON 18 hours, room temperature

PRO T 840524-23-4
NTE stereoselective

RX(23) OF 28 H + P ==> U



U
YIELD 78%

RX(23)

STAGE(1)

CAT 12112-67-3 Iridium, di- μ -chlorobis[(1,2,5,6- η)-1,5-cyclooctadiene]di-, 415918-91-1 Dinaphtho[2,1-d:1',2'-f][1,3,2]dioxaphosphepin-4-amine, N,N-bis[(1R)-1-phenylethyl]-, (11bR)-, 280-57-9 Triethylenediamine
SOL 109-99-9 THF

STAGE(2)

RCT H 62-53-3, P 675608-09-0

CON 15 hours, room temperature

PRO U 840524-24-5

NTE stereoselective

L60 ANSWER 7 OF 44 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 142:431930 CASREACT

TITLE: Selective synthesis of N,N-dimethyl aniline derivatives using dimethyl carbonate as a methylating agent and onium salt as a catalyst

AUTHOR(S): Shivarkar, Anand B.; Gupta, Sunil P.; Chaudhari, Raghunath V.

CORPORATE SOURCE: Homogeneous Catalysis Division, National Chemical Laboratory, Pune, 411008, India

SOURCE: Journal of Molecular Catalysis A: Chemical (2005), 226(1), 49-56

CODEN: JMCCF2; ISSN: 1381-1169

PUBLISHER: Elsevier B.V.

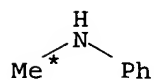
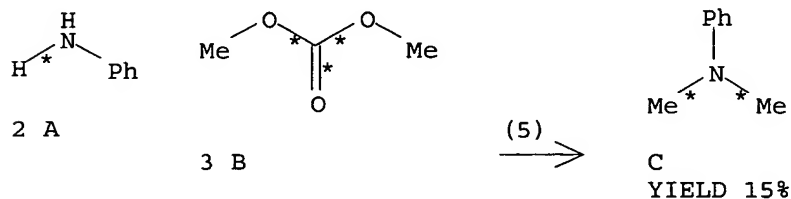
DOCUMENT TYPE: Journal

LANGUAGE: English

AB N-Alkylation of anilines by di-Me carbonate (DMC) catalyzed by onium salts has been demonstrated. The work shows that a simple catalytic system consisting of onium salts in the presence of a small amount of water is extremely effective in enhancing the DMC mediated N-alkylation of anilines to dialkylated products. The effect of reaction conditions, on the synthesis of N,N-di-methylaniline (NNDMA) from aniline and DMC has been investigated. Under the optimized conditions highest yield of NNDMA obtained was 99.8%, which is the best reported for liquid phase N-alkylation of aniline using DMC. The role of water in enhancing the yield of NNDMA is explained and a reaction-networking scheme is constructed, which summarizes the chemical behind liquid phase N-alkylation of anilines by DMC. The catalyst has been shown to recycle up to five times and at the end of fifth recycle almost 98% of NNDMA yields were obtained.

REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

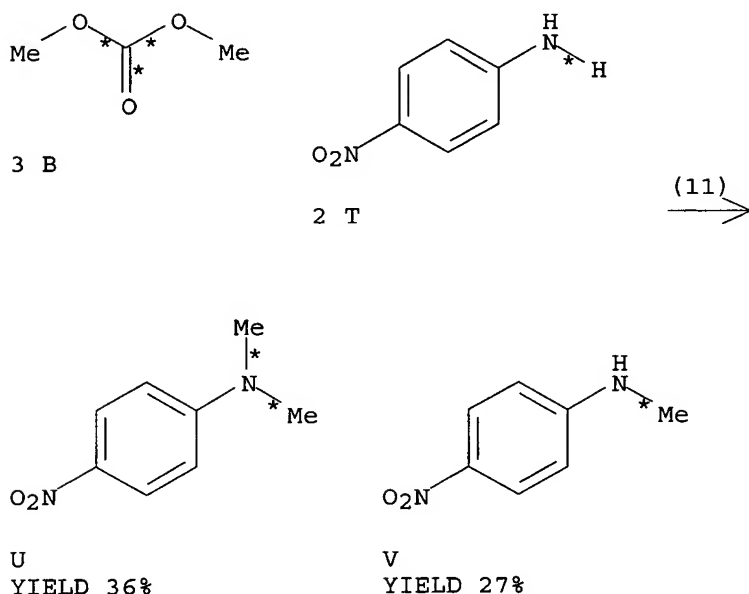
RX(5) OF 19 2 A + 3 B ==> C + H...



H
YIELD 85%

RX(5) RCT A 62-53-3, B 616-38-6
 RGT G 7732-18-5 Water
 PRO C 121-69-7, H 100-61-8
 SOL 616-38-6 Me₂CO₃
 CON 2 hours, 433K, 34 bar
 NTE Cs-Y zeolite used as catalyst, Hast 'C' high pressure Parr reactor used, green chem.-waste redn., high pressure, optimized on catalyst and temp.

RX(11) OF 19 3 B + 2 T ==> U + V



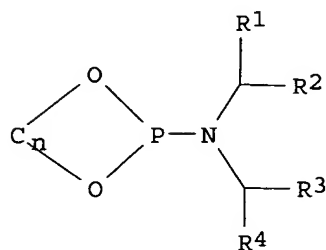
RX(11) RCT B 616-38-6, T 100-01-6
 RGT G 7732-18-5 Water
 PRO U 100-23-2, V 100-15-2
 CAT 71-91-0 Et₄N.Br
 SOL 616-38-6 Me₂CO₃
 CON 2 hours, 443K, 34 bar
 NTE Hast 'C' high pressure Parr reactor used, green chem.-waste redn., high pressure

L60 ANSWER 8 OF 44 CASREACT COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 140:287536 CASREACT
 TITLE: Preparation of phosphoramidite iridium complexes as catalysts for enantioselective amination and etherification reaction
 INVENTOR(S): Hartwig, John F.; Shu, Chutian; Ohmura, Toshimichi; Kiener, Christoph; Lopez, Fernando Garcia
 PATENT ASSIGNEE(S): Yale University, USA
 SOURCE: PCT Int. Appl., 100 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English

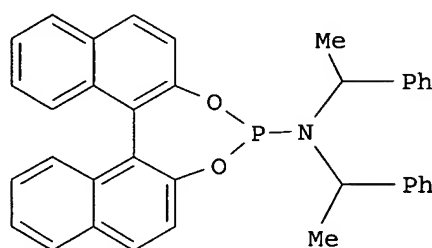
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004024684	A2	20040325	WO 2003-US28718	20030912
WO 2004024684	A3	20040513		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2003272349	A1	20040430	AU 2003-272349	20030912
PRIORITY APPLN. INFO.:			US 2002-410407P	20020913
			US 2003-445154P	20030205
			WO 2003-US28718	20030912

OTHER SOURCE(S): MARPAT 140:287536
GI



I

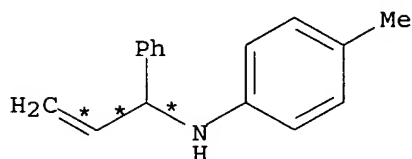
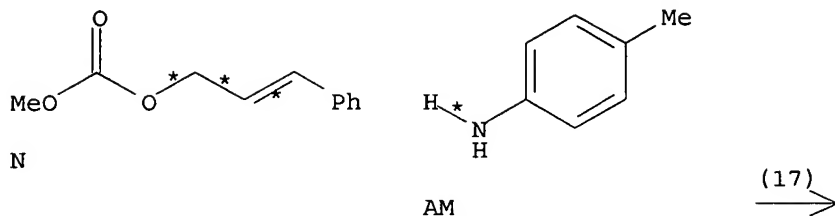


II

AB The present invention is directed to a catalyst composition, comprising: (1) a catalyst precursor having the general structure MSX_n (M = a transition metal selected from the group consisting of iridium, molybdenum, and tungsten; S = a coordinating ligand; X = a counterion; n = 0-5); and (2) a phosphoramidite ligand I (O-Cn-O = aliphatic or aromatic diolate and wherein

R1, R2, R3, and R4 are selected from the group consisting of substituted or unsubstituted aryl groups, substituted or unsubstituted heteroaryl groups, substituted or unsubstituted aliphatic groups, and combinations thereof, with the proviso that at least one of R1, R2, R3, or R4 must be a substituted or unsubstituted aryl or heteroaryl group). The present invention is also directed to activated catalysts made from the above catalyst composition, as well as methods of allylic amination and etherification using the above catalysts. Thus, $[Ir(cod)Cl]_2$ /phosphoramidite ligand II catalyzed enantioselective allylic amination of cinnamyl Me carbonate with benzylamine at room temperature in 10h gave 84% N-(1-phenyl-2-propenyl)benzylamine. The crystal structures of two phosphoramidite iridium complexes were determined

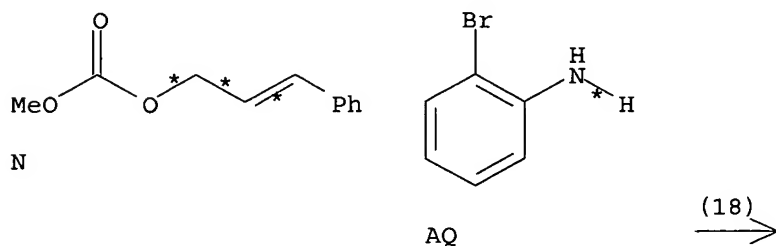
RX(17) OF 54 N + AM ==> AN

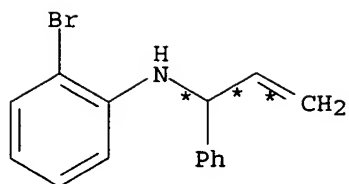


AN
YIELD 76%

RX(17) RCT N 85217-69-2, AM 106-49-0
 RGT AO 280-57-9 Triethylenediamine
 PRO AN 675608-10-3
 CAT 676127-12-1 Dinaphtho[2,1-d:1',2'-f][1,3,2]dioxaphosphepin-4-amine, N,N-bis[(1R)-1-(1-naphthalenyl)ethyl]-, (11bR)-,
 12112-67-3 Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di-
 SOL 109-99-9 THF
 CON 6 hours, room temperature
 NTE stereoselective

RX(18) OF 54 N + AQ ==> AR

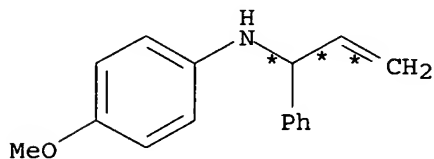
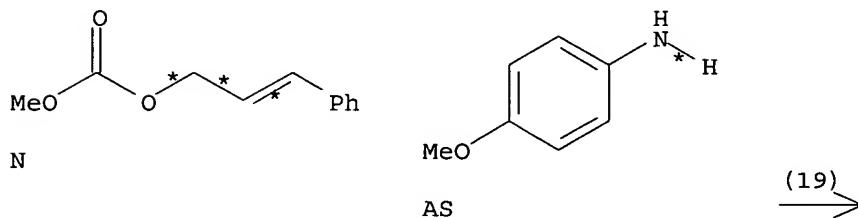




AR
YIELD 66%

RX(18) RCT N 85217-69-2, AQ 615-36-1
RGT AO 280-57-9 Triethylenediamine
PRO AR 675608-11-4
CAT 676127-12-1 Dinaphtho[2,1-d:1',2'-f][1,3,2]dioxaphosphopin-4-amine, N,N-bis[(1R)-1-(1-naphthalenyl)ethyl]-, (11bR)-, 12112-67-3 Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di-
SOL 109-99-9 THF
CON 16 hours, room temperature
NTE stereoselective

RX(19) OF 54 N + AS ==> AT

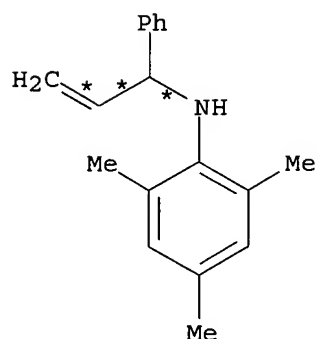
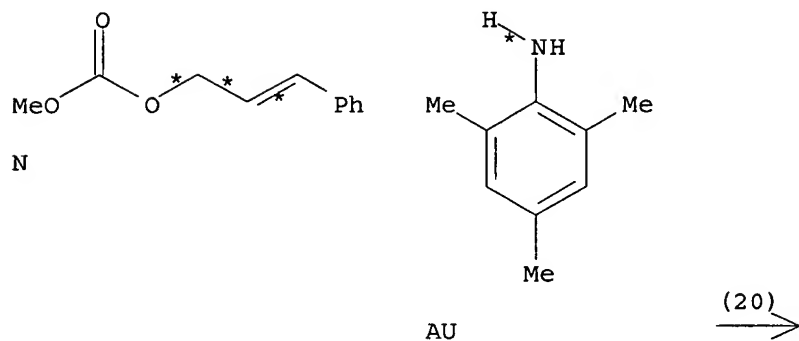


AT
YIELD 91%

RX(19) RCT N 85217-69-2, AS 104-94-9
RGT AO 280-57-9 Triethylenediamine
PRO AT 104937-84-0
CAT 676127-12-1 Dinaphtho[2,1-d:1',2'-f][1,3,2]dioxaphosphopin-4-amine, N,N-bis[(1R)-1-(1-naphthalenyl)ethyl]-, (11bR)-, 12112-67-3 Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di-
SOL 109-99-9 THF

CON 16 hours, room temperature
NTE stereoselective

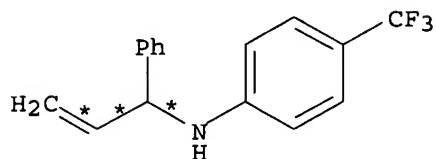
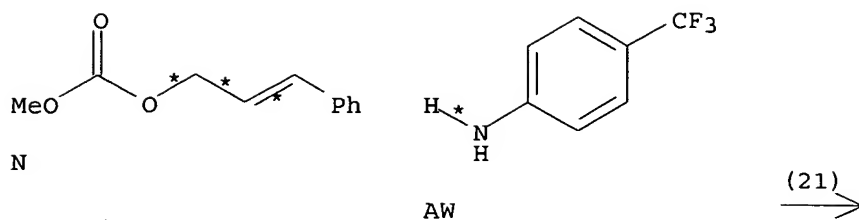
RX(20) OF 54 N + AU ==> AV



AV
YIELD 85%

RX(20) RCT N 85217-69-2, AU 88-05-1
 RGT AO 280-57-9 Triethylenediamine
 PRO AV 675608-12-5
 CAT 676127-12-1 Dinaphtho[2,1-d:1',2'-f][1,3,2]dioxaphosphopin-4-
 amine, N,N-bis[(1R)-1-(1-naphthalenyl)ethyl]-, (11bR)-,
 12112-67-3 Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-
 cyclooctadiene]di-
 SOL 109-99-9 THF
 CON 12 hours, room temperature
 NTE stereoselective

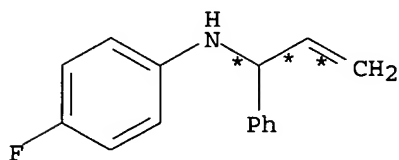
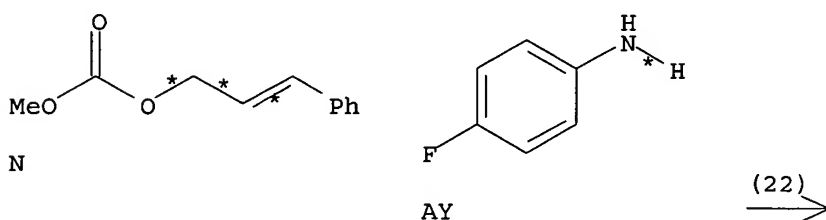
RX(21) OF 54 N + AW ==> AX



AX
YIELD 72%

RX (21) RCT N 85217-69-2, AW 455-14-1
 RGT AO 280-57-9 Triethylenediamine
 PRO AX 675608-13-6
 CAT 676127-12-1 Dinaphtho[2,1-d:1',2'-f][1,3,2]dioxaphosphopin-4-
 amine, N,N-bis[(1R)-1-(1-naphthalenyl)ethyl]-, (11bR)-,
 12112-67-3 Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-
 cyclooctadiene]di-
 SOL 109-99-9 THF
 CON 12 hours, room temperature
 NTE stereoselective

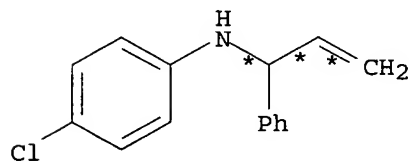
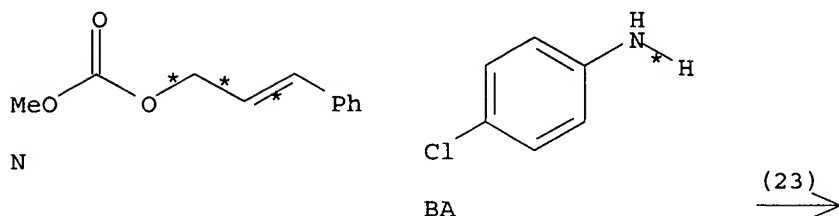
RX (22) OF 54 N + AY ==> AZ



AZ
YIELD 96%

RX(22) RCT N 85217-69-2, AY 371-40-4
 RGT AO 280-57-9 Triethylenediamine
 PRO AZ 675608-14-7
 CAT 676127-12-1 Dinaphtho[2,1-d:1',2'-f][1,3,2]dioxaphosphepin-4-amine, N,N-bis[(1R)-1-(1-naphthalenyl)ethyl]-, (11bR)-, 12112-67-3 Iridium, di- μ -chlorobis[(1,2,5,6- η)-1,5-cyclooctadiene]di-
 SOL 109-99-9 THF
 CON 12 hours, room temperature
 NTE stereoselective

RX(23) OF 54 N + BA ==> BB



BB
 YIELD 95%

RX(23) RCT N 85217-69-2, BA 106-47-8
 RGT AO 280-57-9 Triethylenediamine
 PRO BB 345642-59-3
 CAT 676127-12-1 Dinaphtho[2,1-d:1',2'-f][1,3,2]dioxaphosphepin-4-amine, N,N-bis[(1R)-1-(1-naphthalenyl)ethyl]-, (11bR)-, 12112-67-3 Iridium, di- μ -chlorobis[(1,2,5,6- η)-1,5-cyclooctadiene]di-
 SOL 109-99-9 THF
 CON 16 hours, room temperature
 NTE stereoselective

RX(24) OF 54 N + BC ==> BD

RX(25) RCT N 85217-69-2, BE 536-90-3
 RGT AO 280-57-9 Triethylenediamine
 PRO BF 675608-16-9
 CAT 676127-12-1 Dinaphtho[2,1-d:1',2'-f][1,3,2]dioxaphosphepin-4-amine, N,N-bis[(1R)-1-(1-naphthalenyl)ethyl]-, (11bR)-, 12112-67-3 Iridium, di- μ -chlorobis[(1,2,5,6- η)-1,5-cyclooctadiene]di-
 SOL 109-99-9 THF
 CON 12 hours, room temperature
 NTE stereoselective

L60 ANSWER 9 OF 44 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 141:423999 CASREACT

TITLE: Synthesis of allylic amines: Enantioselective allylation of aromatic amines after in situ generation of an activated cyclometalated iridium catalyst

AUTHOR(S): Shu, Chutian; Leitner, Andreas; Hartwig, John F.

CORPORATE SOURCE: Department of Chemistry, Yale University, New Haven, CT, 06520-8107, USA

SOURCE: Angewandte Chemie, International Edition (2004), 43(36), 4797-4800

CODEN: ACIEF5; ISSN: 1433-7851

PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA

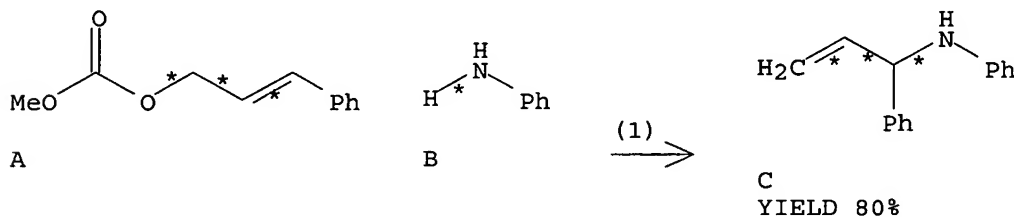
DOCUMENT TYPE: Journal

LANGUAGE: English

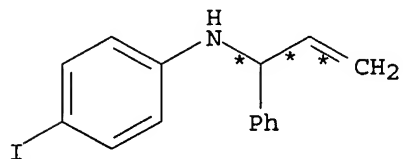
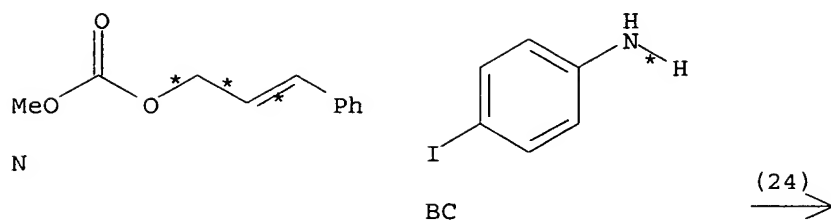
AB Highly regio- and enantioselective allylation of aromatic amines is observed when a cyclometalated Ir-phosphoramidite complex is generated in situ. The active catalyst can be formed from $\{[Ir(cod)Cl]_2\}$ and ligand L with a volatile alkylamine prior to addition of the reagents or upon use of a tertiary amine additive. E.g., a cyclometalated Ir-phosphoramidite complex catalyzed the allylation of PhNH₂ by carbonate (E)-PhCH:CHCH₂OC(O)OMe to give 80% (+)-PhCH(NHPh)CH:CH₂.

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(1) OF 27 A + B ==> C



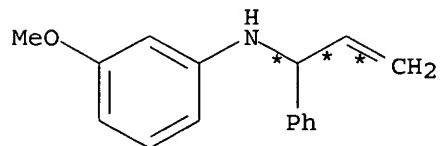
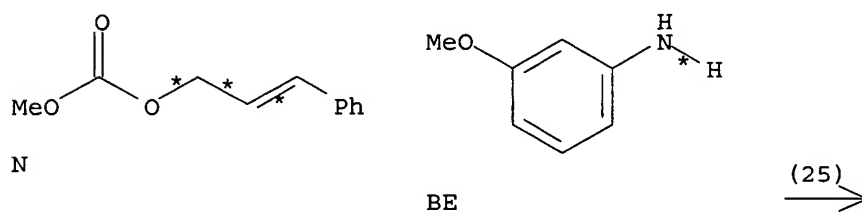
RX(1) RCT A 85217-69-2, B 62-53-3
 PRO C 793726-44-0
 CAT 12112-67-3 Iridium, di- μ -chlorobis[(1,2,5,6- η)-1,5-cyclooctadiene]di-, 676127-12-1 Dinaphtho[2,1-d:1',2'-f][1,3,2]dioxaphosphepin-4-amine, N,N-bis[(1R)-1-(1-naphthalenyl)ethyl]-, (11bR)-
 SOL 109-99-9 THF
 CON 10 hours, room temperature
 NTE in-situ generated catalyst, regioselective, stereoselective



BD
YIELD 92%

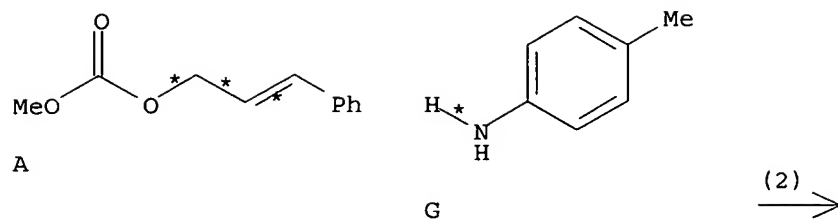
RX(24) RCT N 85217-69-2, BC 540-37-4
 RGT AO 280-57-9 Triethylenediamine
 PRO BD 675608-15-8
 CAT 676127-12-1 Dinaphtho[2,1-d:1',2'-f][1,3,2]dioxaphosphepin-4-amine, N,N-bis[(1R)-1-(1-naphthalenyl)ethyl]-, (11bR)-,
 12112-67-3 Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di-
 SOL 109-99-9 THF
 CON 12 hours, room temperature
 NTE stereoselective

RX(25) OF 54 N + BE ==> BF



BF
YIELD 82%

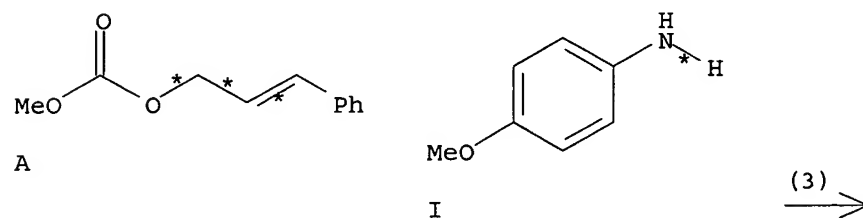
RX(2) OF 27 A + G ==> H

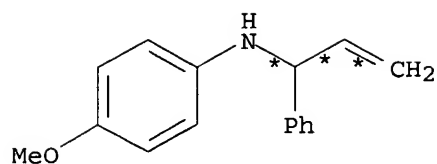


H
YIELD 76%

RX(2) RCT A 85217-69-2, G 106-49-0
 PRO H 793726-45-1
 CAT 12112-67-3 Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di-, 676127-12-1 Dinaphtho[2,1-d:1',2'-f][1,3,2]dioxaphosphepin-4-amine, N,N-bis[(1R)-1-(1-naphthalenyl)ethyl]-, (11bR)-
 SOL 109-99-9 THF
 CON 6 hours, room temperature
 NTE in-situ generated catalyst, regioselective, stereoselective

RX(3) OF 27 A + I ==> J

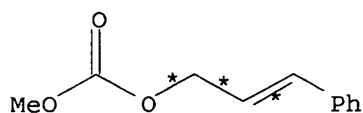




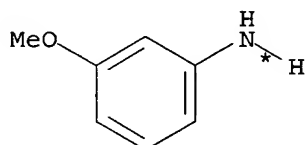
J
YIELD 91%

RX(3) RCT A 85217-69-2, I 104-94-9
 PRO J 793726-47-3
 CAT 12112-67-3 Iridium, di- μ -chlorobis[(1,2,5,6- η)-1,5-cyclooctadiene]di-, 676127-12-1 Dinaphtho[2,1-d:1',2'-f][1,3,2]dioxaphosphepin-4-amine, N,N-bis[(1R)-1-(1-naphthalenyl)ethyl]-, (11bR)-
 SOL 109-99-9 THF
 CON 4 hours, room temperature
 NTE in-situ generated catalyst, regioselective, stereoselective

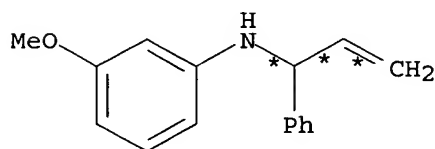
RX(4) OF 27 A + K ==> L



A

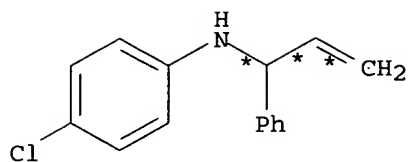


K



L
YIELD 82%

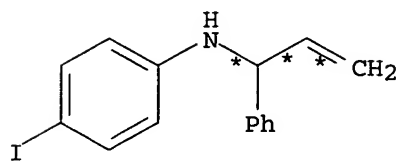
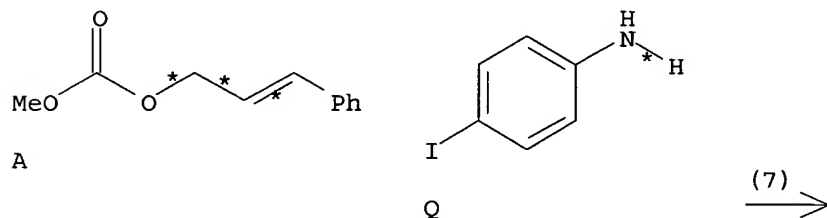
RX(4) RCT A 85217-69-2, K 536-90-3
 PRO L 793726-48-4
 CAT 12112-67-3 Iridium, di- μ -chlorobis[(1,2,5,6- η)-1,5-cyclooctadiene]di-, 676127-12-1 Dinaphtho[2,1-d:1',2'-f][1,3,2]dioxaphosphepin-4-amine, N,N-bis[(1R)-1-(1-naphthalenyl)ethyl]-, (11bR)-
 SOL 109-99-9 THF
 CON 4 hours, room temperature
 NTE in-situ generated catalyst, regioselective, stereoselective



P
YIELD 89%

RX(6) RCT A 85217-69-2, O 106-47-8
 PRO P 793726-52-0
 CAT 12112-67-3 Iridium, di- μ -chlorobis[(1,2,5,6- η)-1,5-cyclooctadiene]di-, 676127-12-1 Dinaphtho[2,1-d:1',2'-f][1,3,2]dioxaphosphepin-4-amine, N,N-bis[(1R)-1-(1-naphthalenyl)ethyl]-, (11bR)-
 SOL 109-99-9 THF
 CON 10 hours, room temperature
 NTE in-situ generated catalyst, regioselective, stereoselective

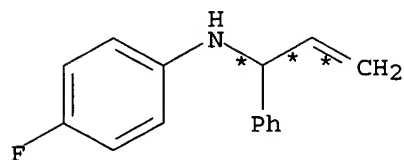
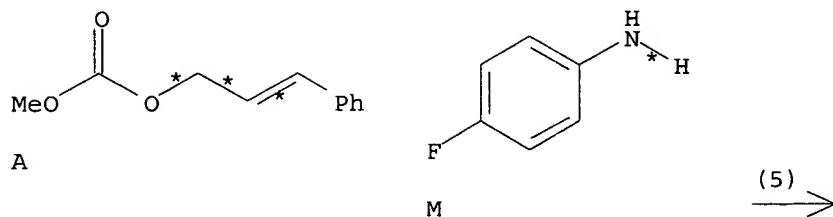
RX(7) OF 27 A + Q ==> R



R
YIELD 92%

RX(7) RCT A 85217-69-2, Q 540-37-4
 PRO R 793726-53-1
 CAT 12112-67-3 Iridium, di- μ -chlorobis[(1,2,5,6- η)-1,5-cyclooctadiene]di-, 676127-12-1 Dinaphtho[2,1-d:1',2'-f][1,3,2]dioxaphosphepin-4-amine, N,N-bis[(1R)-1-(1-naphthalenyl)ethyl]-, (11bR)-
 SOL 109-99-9 THF
 CON 10 hours, room temperature
 NTE in-situ generated catalyst, regioselective, stereoselective

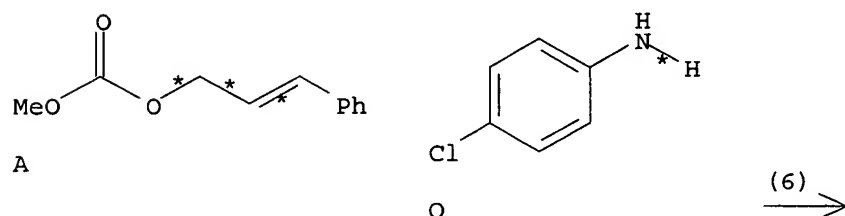
RX(5) OF 27 A + M ==> N



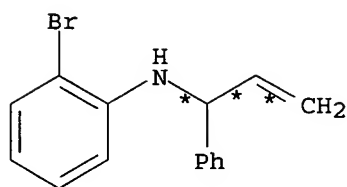
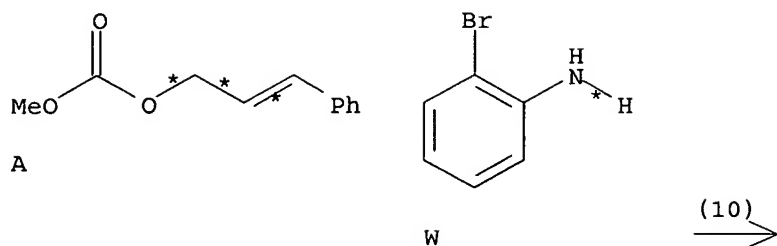
N
YIELD 90%

RX(5) RCT A 85217-69-2, M 371-40-4
 PRO N 793726-51-9
 CAT 12112-67-3 Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di-, 676127-12-1 Dinaphtho[2,1-d:1',2'-f][1,3,2]dioxaphosphopin-4-amine, N,N-bis[(1R)-1-(1-naphthalenyl)ethyl]-, (11bR)-
 SOL 109-99-9 THF
 CON 10 hours, room temperature
 NTE in-situ generated catalyst, regioselective, stereoselective

RX(6) OF 27 A + O ==> P



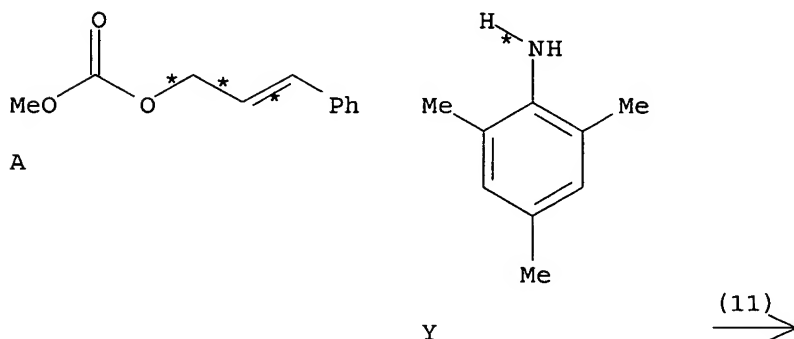
RX(10) OF 27 A + W ==> X

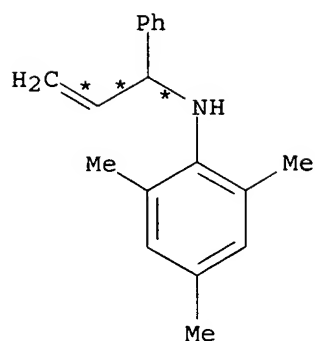


X
YIELD 66%

RX(10) RCT A 85217-69-2, W 615-36-1
 PRO X 793726-57-5
 CAT 12112-67-3 Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di-, 676127-12-1 Dinaphtho[2,1-d:1',2'-f][1,3,2]dioxaphosphepin-4-amine, N,N-bis[(1R)-1-(1-naphthalenyl)ethyl]-, (11bR)-
 SOL 109-99-9 THF
 CON 16 hours, room temperature
 NTE in-situ generated catalyst, regioselective, stereoselective

RX(11) OF 27 A + Y ==> Z

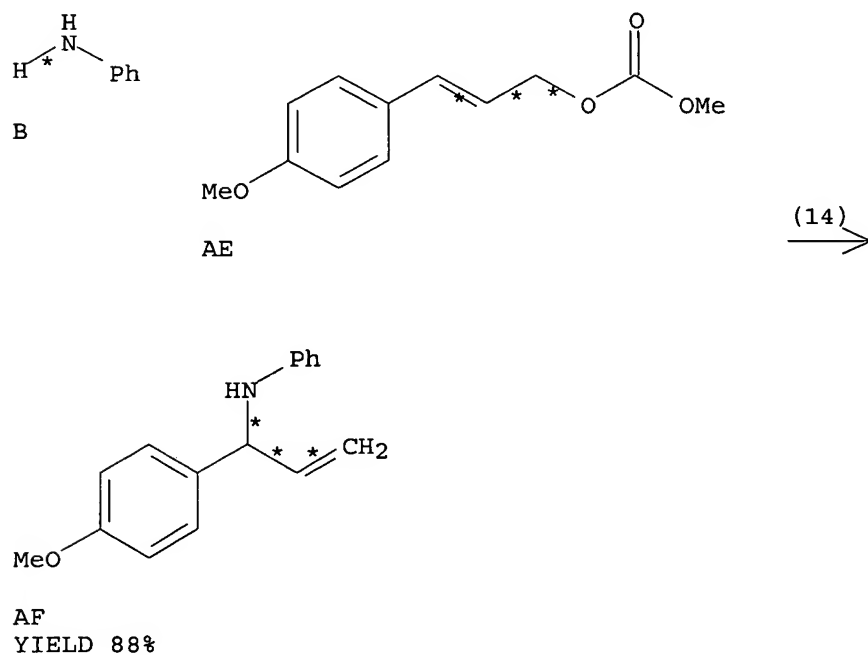




Z
YIELD 82%

RX(11) RCT A 85217-69-2, Y 88-05-1
 PRO Z 793726-58-6
 CAT 12112-67-3 Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di-, 676127-12-1 Dinaphtho[2,1-d:1',2'-f][1,3,2]dioxaphosphepin-4-amine, N,N-bis[(1R)-1-(1-naphthalenyl)ethyl]-, (11bR)-
 SOL 109-99-9 THF
 CON 2 hours, room temperature
 NTE in-situ generated catalyst, regioselective, stereoselective

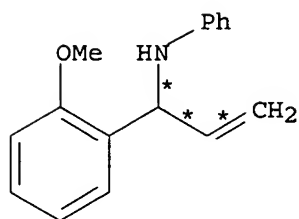
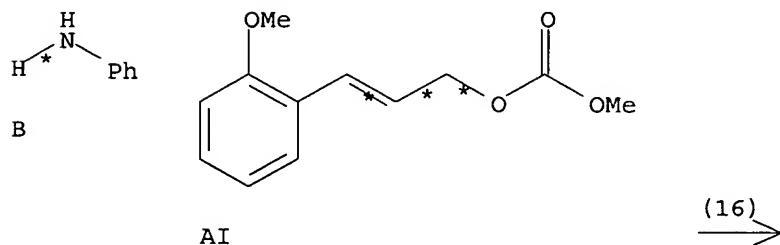
RX(14) OF 27 B + AE ==> AF



RX(14) RCT B 62-53-3, AE 496789-06-1
 PRO AF 793726-64-4

CAT 12112-67-3 Iridium, di- μ -chlorobis[(1,2,5,6- η)-1,5-cyclooctadiene]di-, 676127-12-1 Dinaphtho[2,1-d:1',2'-f][1,3,2]dioxaphosphepin-4-amine, N,N-bis[(1R)-1-(1-naphthalenyl)ethyl]-, (11bR)-
 SOL 109-99-9 THF
 CON 10 hours, room temperature
 NTE in-situ generated catalyst, regioselective, stereoselective

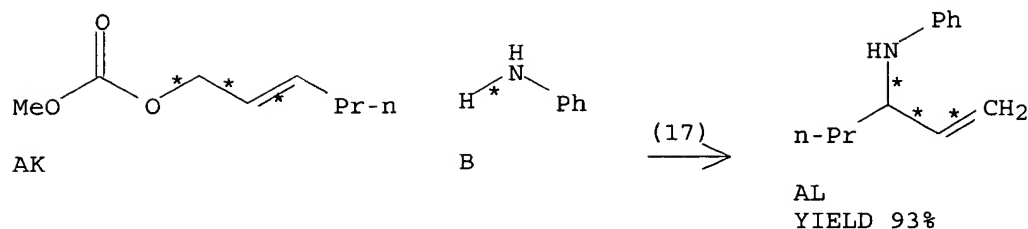
RX(16) OF 27 B + AI ==> AJ



AJ
 YIELD 91%

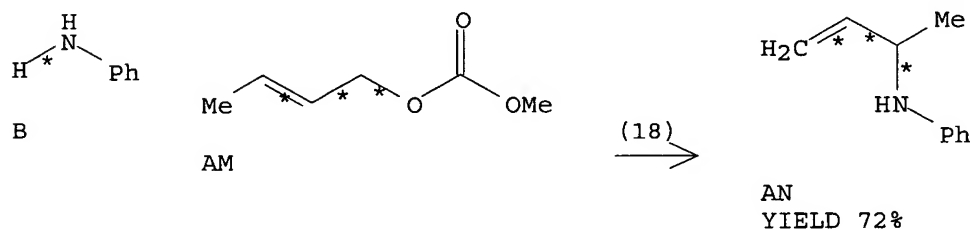
RX(16) RCT B 62-53-3, AI 512789-12-7
 PRO AJ 793726-66-6
 CAT 12112-67-3 Iridium, di- μ -chlorobis[(1,2,5,6- η)-1,5-cyclooctadiene]di-, 676127-12-1 Dinaphtho[2,1-d:1',2'-f][1,3,2]dioxaphosphepin-4-amine, N,N-bis[(1R)-1-(1-naphthalenyl)ethyl]-, (11bR)-
 SOL 109-99-9 THF
 CON 10 hours, room temperature
 NTE in-situ generated catalyst, regioselective, stereoselective

RX(17) OF 27 AK + B ==> AL



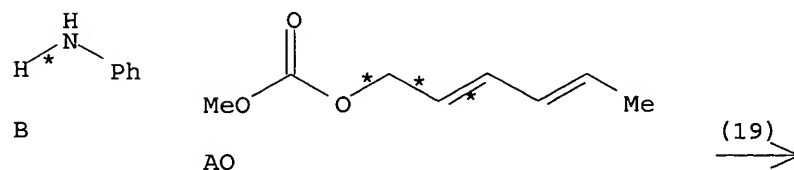
RX(17) RCT AK 107574-36-7, B 62-53-3
 PRO AL 793726-67-7
 CAT 12112-67-3 Iridium, di- μ -chlorobis[(1,2,5,6- η)-1,5-cyclooctadiene]di-, 676127-12-1 Dinaphtho[2,1-d:1',2'-f][1,3,2]dioxaphosphepin-4-amine, N,N-bis[(1R)-1-(1-naphthalenyl)ethyl]-, (11bR)-
 SOL 109-99-9 THF
 CON 2.5 hours, room temperature
 NTE in-situ generated catalyst, regioselective, stereoselective

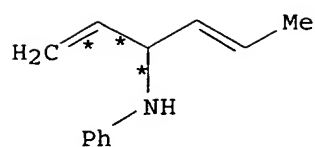
RX(18) OF 27 B + AM ==> AN



RX(18) RCT B 62-53-3, AM 103185-13-3
 PRO AN 70094-92-7
 CAT 12112-67-3 Iridium, di- μ -chlorobis[(1,2,5,6- η)-1,5-cyclooctadiene]di-, 676127-12-1 Dinaphtho[2,1-d:1',2'-f][1,3,2]dioxaphosphepin-4-amine, N,N-bis[(1R)-1-(1-naphthalenyl)ethyl]-, (11bR)-
 SOL 109-99-9 THF
 CON 3 hours, room temperature
 NTE in-situ generated catalyst, regioselective, stereoselective

RX(19) OF 27 B + AO ==> AP



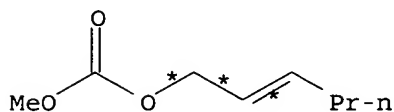


AP

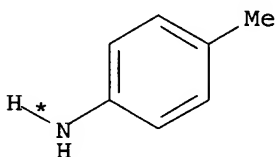
YIELD 87%

RX(19) RCT B 62-53-3, AO 675608-09-0
 PRO AP 793726-69-9
 CAT 12112-67-3 Iridium, di- μ -chlorobis[(1,2,5,6- η)-1,5-cyclooctadiene]di-, 676127-12-1 Dinaphtho[2,1-d:1',2'-f][1,3,2]dioxaphosphepin-4-amine, N,N-bis[(1R)-1-(1-naphthalenyl)ethyl]-, (11bR)-
 SOL 109-99-9 THF
 CON 3 hours, room temperature
 NTE in-situ generated catalyst, regioselective, stereoselective

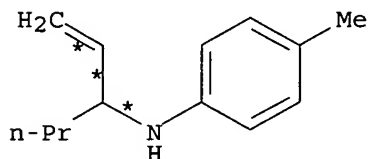
RX(20) OF 27 AK + G ==> AQ



AK



G

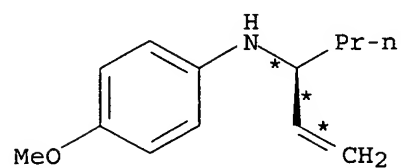
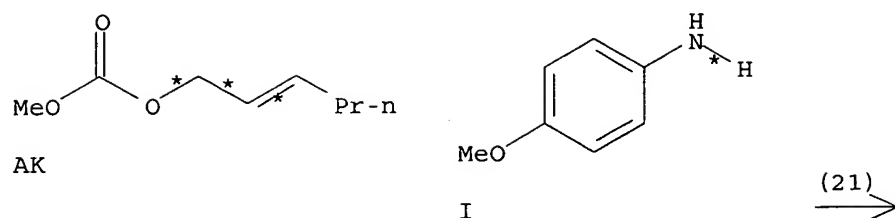


AQ

YIELD 94%

RX(20) RCT AK 107574-36-7, G 106-49-0
 PRO AQ 793726-46-2
 CAT 12112-67-3 Iridium, di- μ -chlorobis[(1,2,5,6- η)-1,5-cyclooctadiene]di-, 415918-91-1 Dinaphtho[2,1-d:1',2'-f][1,3,2]dioxaphosphepin-4-amine, N,N-bis[(1R)-1-phenylethyl]-, (11bR)-
 SOL 109-99-9 THF
 CON 2 hours, room temperature
 NTE in-situ generated catalyst, regioselective, stereoselective

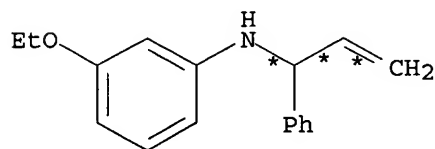
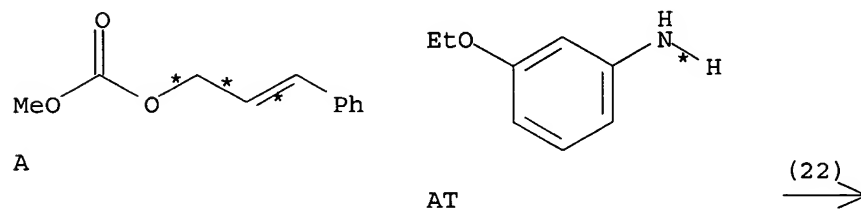
RX(21) OF 27 AK + I ==> AS



YIELD 95%

RX(21) RCT AK 107574-36-7, I 104-94-9
 PRO AS 562870-91-1
 CAT 12112-67-3 Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di-, 415918-91-1 Dinaphtho[2,1-d:1',2'-f][1,3,2]dioxaphosphepin-4-amine, N,N-bis[(1R)-1-phenylethyl]-, (11bR)-
 SOL 109-99-9 THF
 CON 2 hours, room temperature
 NTE in-situ generated catalyst, regioselective, stereoselective

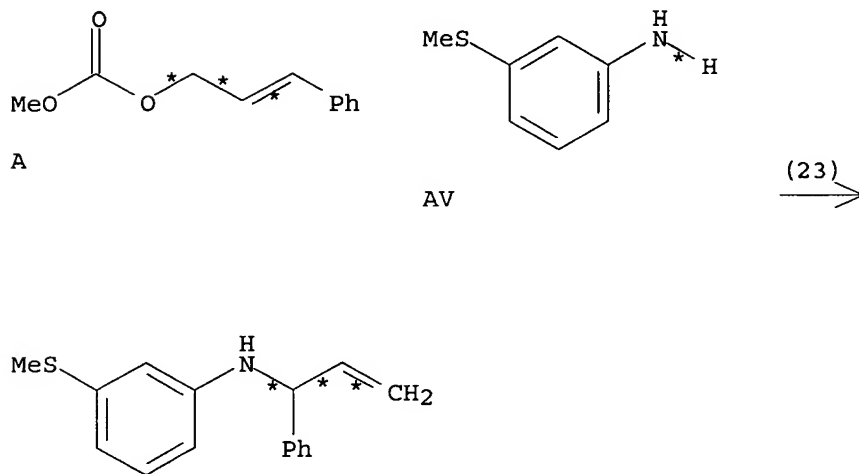
RX(22) OF 27 A + AT ==> AU



YIELD 86%

RX(22) RCT A 85217-69-2, AT 621-33-0
 PRO AU 793726-50-8
 CAT 12112-67-3 Iridium, di- μ -chlorobis[(1,2,5,6- η)-1,5-cyclooctadiene]di-, 415918-91-1 Dinaphtho[2,1-d:1',2'-f][1,3,2]dioxaphosphepin-4-amine, N,N-bis[(1R)-1-phenylethyl]-, (11bR)-
 SOL 109-99-9 THF
 CON 2.5 hours, room temperature
 NTE in-situ generated catalyst, regioselective, stereoselective

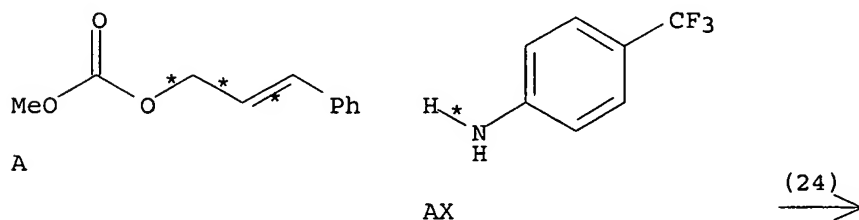
RX(23) OF 27 A + AV ==> AW

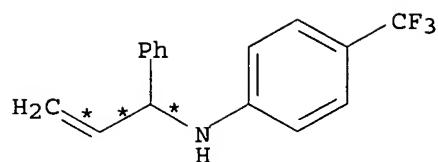


AW
 YIELD 85%

RX(23) RCT A 85217-69-2, AV 1783-81-9
 PRO AW 793726-59-7
 CAT 12112-67-3 Iridium, di- μ -chlorobis[(1,2,5,6- η)-1,5-cyclooctadiene]di-, 415918-91-1 Dinaphtho[2,1-d:1',2'-f][1,3,2]dioxaphosphepin-4-amine, N,N-bis[(1R)-1-phenylethyl]-, (11bR)-
 SOL 109-99-9 THF
 CON 2.5 hours, room temperature
 NTE in-situ generated catalyst, regioselective, stereoselective

RX(24) OF 27 A + AX ==> AY

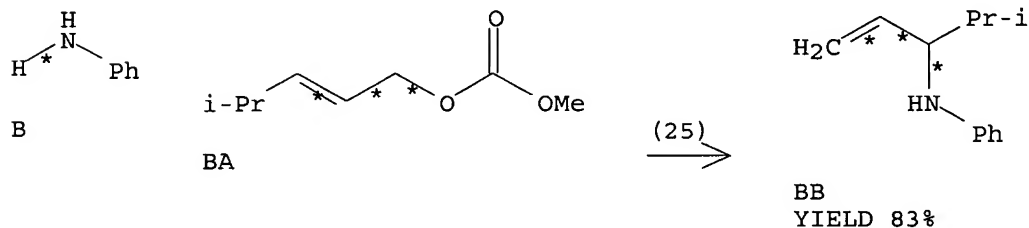




AY
YIELD 72%

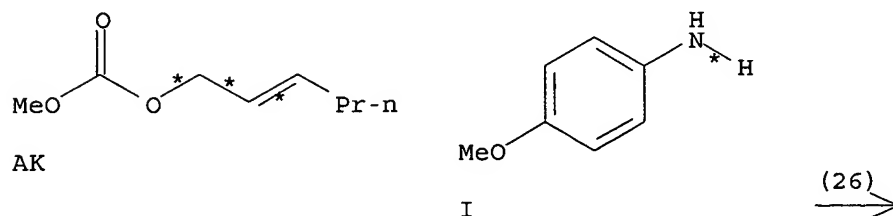
RX(24)	RCT	A 85217-69-2, AX 455-14-1
	PRO	AY 793726-56-4
	CAT	12112-67-3 Iridium, di- μ -chlorobis[(1,2,5,6- η)-1,5-cyclooctadiene]di-, 676127-12-1 Dinaphtho[2,1-d:1',2'-f][1,3,2]dioxaphosphepin-4-amine, N,N-bis[(1R)-1-(1-naphthalenyl)ethyl]-, (11bR)-, 280-57-9 Triethylenediamine
	SOL	109-99-9 THF
	CON	16 hours, room temperature
	NTE	in-situ generated catalyst, regioselective, stereoselective

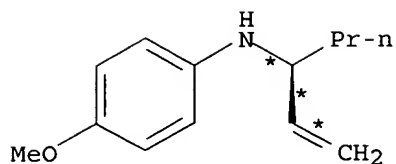
RX (25) OF 27 B + BA ==> BB



RX(25)	RCT	B 62-53-3, BA 675608-08-9
	PRO	BB 793726-70-2
	CAT	12112-67-3 Iridium, di- μ -chlorobis[(1,2,5,6- η)-1,5-cyclooctadiene]di-, 676127-12-1 Dinaphtho[2,1-d:1',2'-f][1,3,2]dioxaphosphepin-4-amine, N,N-bis[(1R)-1-(1-naphthalenyl)ethyl]-, (11bR)-, 280-57-9 Triethylenediamine
	SOL	109-99-9 THF
	CON	16 hours, room temperature
	NTE	in-situ generated catalyst, regioselective, stereoselective

RX (26) OF 27 AK + I ==> AS

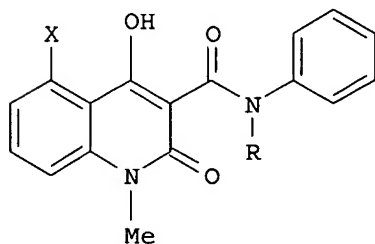




AS
YIELD 85%

RX(26) RCT AK 107574-36-7, I 104-94-9
 PRO AS 562870-91-1
 CAT 12112-67-3 Iridium, di-μ-chlorobis[(1,2,5,6-η)-1,5-cyclooctadiene]di-, 676127-12-1 Dinaphtho[2,1-d:1',2'-f][1,3,2]dioxaphosphepin-4-amine, N,N-bis[(1R)-1-(1-naphthalenyl)ethyl]-, (11bR)-, 280-57-9 Triethylenediamine
 SOL 109-99-9 THF
 CON 50 deg C
 NTE in-situ generated catalyst, regioselective, stereoselective

L60 ANSWER 10 OF 44 CASREACT COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 140:287248 CASREACT
 TITLE: Synthesis and Biological Evaluation of New 1,2-Dihydro-4-hydroxy-2-oxo-3-quinolinecarboxamides for Treatment of Autoimmune Disorders: Structure-Activity Relationship
 AUTHOR(S): Joensson, Stig; Andersson, Gunnar; Fex, Tomas; Fristedt, Tomas; Hedlund, Gunnar; Jansson, Karl; Abramo, Lisbeth; Fritzson, Ingela; Pekarski, Olga; Runstroem, Anna; Sandin, Helena; Thuvesson, Ingela; Bjoerk, Anders
 CORPORATE SOURCE: Active Biotech Research AB, Lund, SE-220 07, Swed.
 SOURCE: Journal of Medicinal Chemistry (2004), 47(8), 2075-2088
 CODEN: JMCMAR; ISSN: 0022-2623
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



I

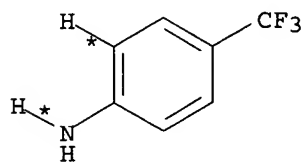
AB Roquinimex-related 3-quinolinecarboxamide derivs., e.g. I (R = Et, X = Cl), were prepared and evaluated for treatment of autoimmune disorders. The

comps. were tested in mice for their inhibitory effects on disease development in the acute exptl. autoimmune encephalomyelitis model and selected comps. in the beagle dog for induction of proinflammatory reaction. Structure-activity relationships are discussed. Compound I (R = Et, X = Cl), laquinimod, showed improved potency and superior toxicol. profile compared to the lead compound roquinimex (I; R = Me, X = H) and was selected for clin. studies (currently in phase II).

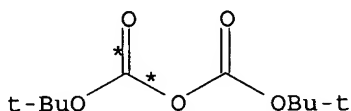
REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(173) OF 182 COMPOSED OF RX(94), RX(95)

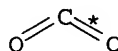
RX(173) BR + BC + BA + C + AH ==> FW



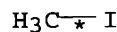
BR



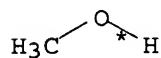
BC



BA

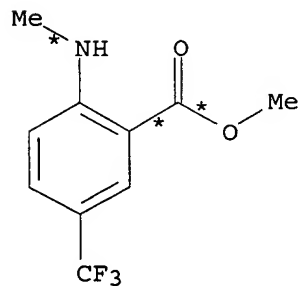


C



AH

2
STEPS
→



FW

RX(94) RCT BR 455-14-1, BC 24424-99-5

STAGE(1)

SOL 109-99-9 THF

CON 18 hours, reflux

STAGE(2)

RGT BD 594-19-4 t-BuLi

SOL 109-99-9 THF, 110-54-3 Hexane

CON 2.5 hours, -40 deg C

STAGE(3)

RCT BA 124-38-9
CON SUBSTAGE(1) -40 deg C
SUBSTAGE(2) -40 deg C -> 0 deg C

STAGE(4)
RGT G 7732-18-5 Water
CON 0 deg C

PRO FV 141940-29-6
NTE regioselective

RX(95) RCT FV 141940-29-6

STAGE(1)
RGT F 7646-69-7 NaH
SOL 68-12-2 DMF
CON 1 hour, 0 deg C

STAGE(2)
RCT C 74-88-4
CON SUBSTAGE(1) 0 deg C
SUBSTAGE(2) overnight, room temperature

STAGE(3)
RGT G 7732-18-5 Water

STAGE(4)
RCT AH 67-56-1
RGT AD 7647-01-0 HCl
SOL 7732-18-5 Water, 67-56-1 MeOH
CON overnight, room temperature

STAGE(5)
RGT BE 1310-73-2 NaOH
SOL 7732-18-5 Water

PRO FW 675575-41-4

L60 ANSWER 11 OF 44 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 140:289172 CASREACT

TITLE: Carbamate Synthesis on Pd/C Catalysts: Gas-Solid versus Slurry Processes

AUTHOR(S): Toochinda, Pisanu; Chuang, Steven S. C.

CORPORATE SOURCE: Department of Chemical Engineering, The University of Akron, Akron, OH, 44325-3906, USA

SOURCE: Industrial & Engineering Chemistry Research (2004), 43(5), 1192-1199

CODEN: IECRED; ISSN: 0888-5885

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

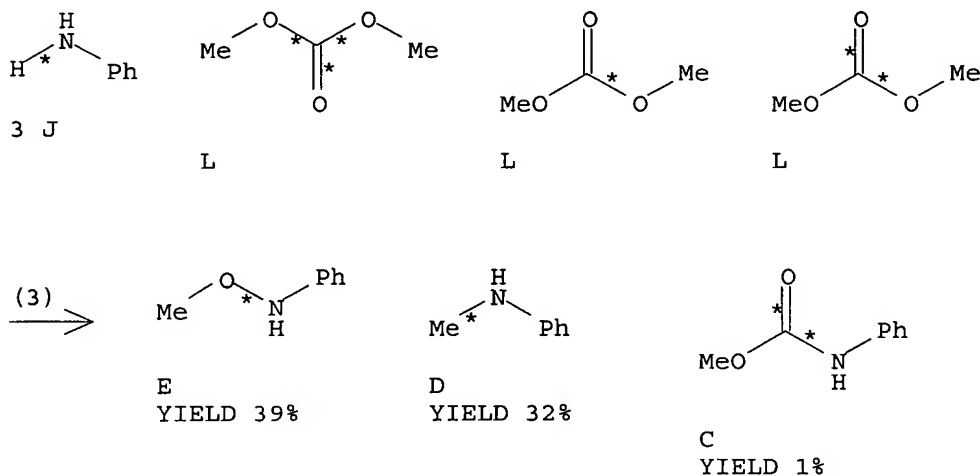
LANGUAGE: English

AB Carbamate synthesis has been studied over NaI-Pd/C in slurry, gas-solid, and tubular reactors at 373-438 K and 0.41-7.61 MPa. The gas-solid carbamate synthesis process in which the CO, O₂, methanol, and aniline reactants are present in the gas phase and the catalyst is in solid form occurs at a significantly higher rate than the slurry-phase synthesis in which CO and O₂ dissolve in the liquid methanol/aniline mixture. The high rate of the gas-solid carbamate synthesis compared with that of the slurry-phase synthesis can be attributed to (i) the intimate contact

between the NaI promoter and the Pd on the carbon surface, (ii) the absence of solubility limitations in the gas-solid synthesis, and (iii) the slowing of the sintering of the Pd particles. Reaction pathway studies show that the direct oxidative carbonylation of aniline with methanol is the most effective pathway for carbamate synthesis. A low-cost, environmentally benign carbamate synthesis for the replacement of the isocyanate synthesis from phosgene/amine can be developed by coupling the high rate of the gas-solid synthesis with its intrinsic advantage of ease of catalyst recovery.

REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(3) OF 5 3 J + 3 L ==> E + D + C



RX(3) RCT J 62-53-3, L 616-38-6
 PRO E 32654-23-2, D 100-61-8, C 2603-10-3
 CAT 7681-82-5 NaI, 7440-05-3 Pd, 7440-44-0 Carbon
 CON 480 minutes, 453K, 2.42 MPa
 NTE thermal, Fixed bed reactor used, alternative reaction conditions
 (slurry method) gave lower yield, alternative reaction
 conditions shown, high pressure

L60 ANSWER 12 OF 44 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 141:71421 CASREACT

TITLE: Zirconium catalyzed enantioselective hydroamination/cyclization

AUTHOR(S): Knight, Paul D.; Munslow, Ian; O'Shaughnessy, Paul N.; Scott, Peter

CORPORATE SOURCE: Department of Chemistry, University of Warwick, Coventry, UK

SOURCE: Chemical Communications (Cambridge, United Kingdom) (2004), (7), 894-895

CODEN: CHCOFS; ISSN: 1359-7345

PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

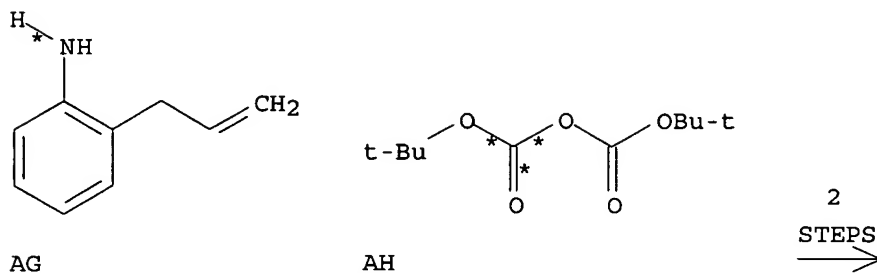
AB A chiral zirconium alkyl cation catalyzes the cyclization of certain aminoalkenes with enantioselectivity up to 82%, the highest thus far observed

for such a process.

REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(23) OF 26 COMPOSED OF RX(12), RX(5)

RX(23) AG + AH ==> S



S
YIELD 59%

RX(12) RCT AG 32704-22-6, AH 24424-99-5
RGT AI 121-44-8 Et₃N
PRO R 309974-70-7
SOL 109-99-9 THF
CON 1 day, reflux

RX(5) RCT R 309974-70-7

STAGE(1)
RGT H 16853-85-3 LiAlH₄
SOL 109-99-9 THF
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) 1 day, reflux
SUBSTAGE(3) reflux -> 0 deg C

STAGE(2)
RGT K 7732-18-5 Water
CON 0 deg C

PRO S 41652-73-7

160 ANSWER 13 OF 44 CASREACT COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 141:277290 CASREACT

TITLE: Selective N,N-dimethylation of primary aromatic amines with dimethyl carbonate in the presence of diphenylammonium triflate

AUTHOR(S): Shen, Zhen Lu; Jiang, Xuan Zhen

CORPORATE SOURCE: Department of Chemistry, Zhejiang University, Hangzhou, Zhejiang, 310027, Peop. Rep. China

SOURCE: Journal of Molecular Catalysis A: Chemical (2004), 213(2), 193-198
CODEN: JMCCF2; ISSN: 1381-1169

PUBLISHER: Elsevier Science B.V.

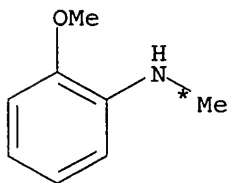
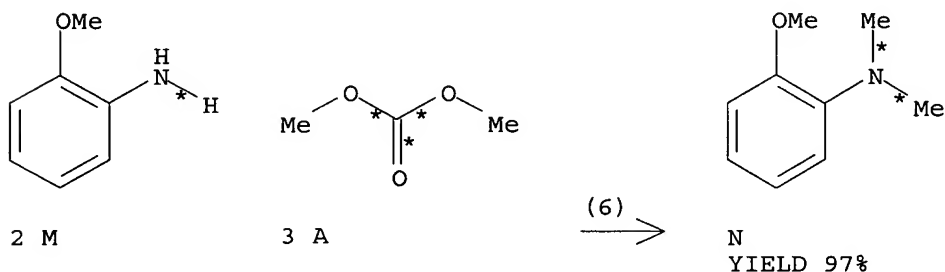
DOCUMENT TYPE: Journal

LANGUAGE: English

AB A facile synthesis of N,N-dimethylanilines from primary aromatic amines and di-Me carbonate has been achieved for the first time in the presence of diphenylammonium triflate. N,N-Dimethylanilines were selectively obtained in high yields. All the reaction parameters, viz. reaction temperature, time, molar ratio of reactants, and catalyst amount, were examined in the reaction of aniline and di-Me carbonate. The conversion of aniline and the selectivity to N,N-dimethylaniline were 99.9 and 99.6%, resp., at 180° in 160 min.

REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

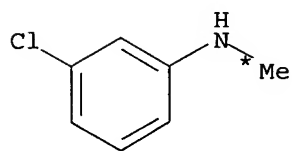
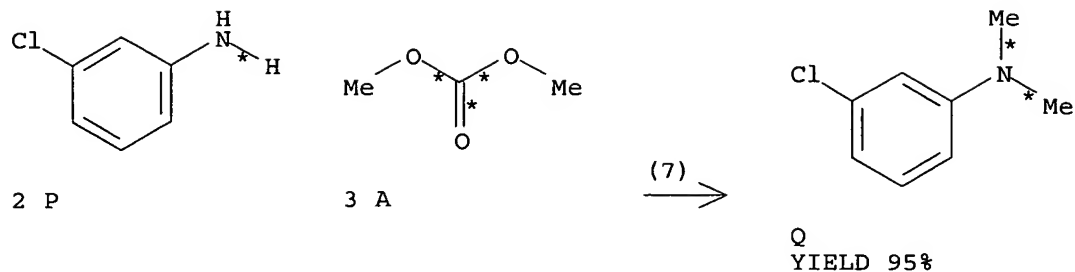
RX(6) OF 11 2 M + 3 A ==> N + O



O

RX(6) RCT M 90-04-0, A 616-38-6
PRO N 700-75-4, O 10541-78-3
CAT 164411-06-7 Methanesulfonic acid, trifluoro-, compd. with N-phenylbenzenamine (1:1)
CON SUBSTAGE(1) 230 minutes, 180 deg C
SUBSTAGE(2) 180 deg C -> room temperature
NTE chemoselective, thermal, autoclave used, green chem.-waste redn., no solvent, other product(s) also detected

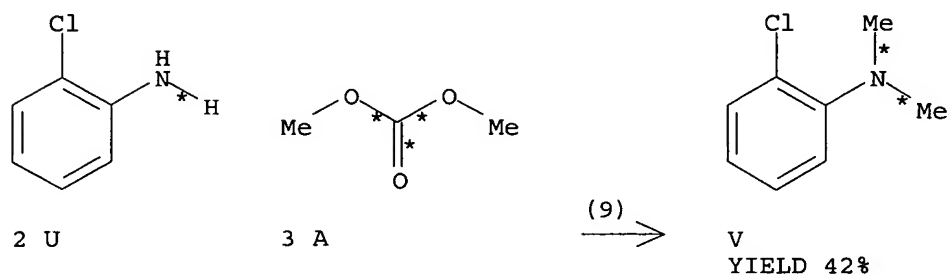
RX(7) OF 11 2 P + 3 A ==> Q + R

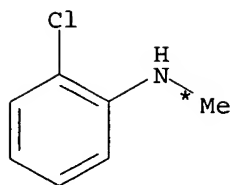


R

RX(7) RCT P 108-42-9, A 616-38-6
 PRO Q 6848-13-1, R 7006-52-2
 CAT 164411-06-7 Methanesulfonic acid, trifluoro-, compd. with
 N-phenylbenzenamine (1:1)
 CON SUBSTAGE(1) 300 minutes, 180 deg C
 SUBSTAGE(2) 180 deg C -> room temperature
 NTE chemoselective, thermal, autoclave used, green chem.-waste
 redn., no solvent, other product(s) also detected

RX(9) OF 11 2 U + 3 A ==> V + W





W

RX(9) RCT U 95-51-2, A 616-38-6
 PRO V 698-01-1, W 932-32-1
 CAT 164411-06-7 Methanesulfonic acid, trifluoro-, compd. with
 N-phenylbenzenamine (1:1)
 CON SUBSTAGE(1) 300 minutes, 180 deg C
 SUBSTAGE(2) 180 deg C -> room temperature
 NTE chemoselective, thermal, autoclave used, green chem.-waste
 redn., no solvent, other product(s) also detected

L60 ANSWER 14 OF 44 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 142:55972 CASREACT

TITLE: Carbomethoxylating reactivity of methyl phenyl
 carbonate toward aromatic amines in the presence of
 group 3 metal (Sc, La) triflate catalysts

AUTHOR(S): Distaso, Monica; Quaranta, Eugenio

CORPORATE SOURCE: Dipartimento di Chimica, Universita di Bari, Bari,
 70126, Italy

SOURCE: Journal of Catalysis (2004), 228(1), 36-42
 CODEN: JCTLA5; ISSN: 0021-9517

PUBLISHER: Elsevier

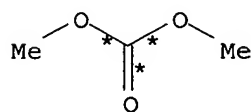
DOCUMENT TYPE: Journal

LANGUAGE: English

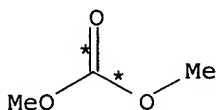
AB MeOCO₂Ph (I) has been investigated as a carbomethoxylating agent for aromatic amines in the presence of Sc or La triflate catalysts. Under mild conditions (363 K), both Sc(OTf)₃ and La(OTf)₃ (OTf = O₃SCF₃) promote the carbamation of aniline and some industrially relevant aromatic diamines, such as 4,4'-methylenedianiline and 2,4-diaminotoluene, with I. Carbamate yield and selectivity are markedly affected by the exptl. conditions (temperature, reaction medium, nature of the metal center). Sc(OTf)₃ is a more effective and selective carbamation catalyst than La(OTf)₃. Ad hoc expts. have shown that, in the presence of the M(OTf)₃ (M = Sc, La) catalysts, I is not only more reactive but also a more selective carbomethoxylating agent than (MeO)₂CO.

REFERENCE COUNT: 42 THERE ARE 42 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

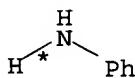
RX(2) OF 12 4 G + 3 B ==> C + D + H



3 G

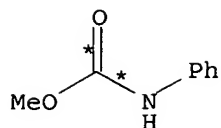


G

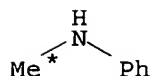


3 B

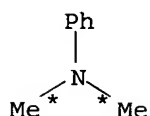




C
YIELD 3%



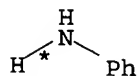
D
YIELD 20%



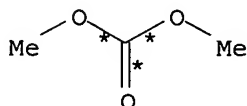
H
YIELD 5%

RX(2) RCT G 616-38-6, B 62-53-3
 PRO C 2603-10-3, D 100-61-8, H 121-69-7
 CAT 52093-26-2 Methanesulfonic acid, trifluoro-, lanthanum(3+) salt
 CON SUBSTAGE(1) 24 hours, 368K
 SUBSTAGE(2) 368K -> room temperature
 NTE no solvent

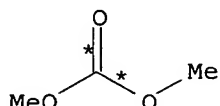
RX(3) OF 12 3 B + 4 G ==> C + D + H



3 B

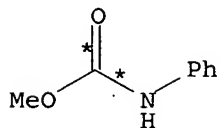


3 G

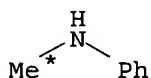


G

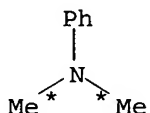
(3) →



C
YIELD 18%



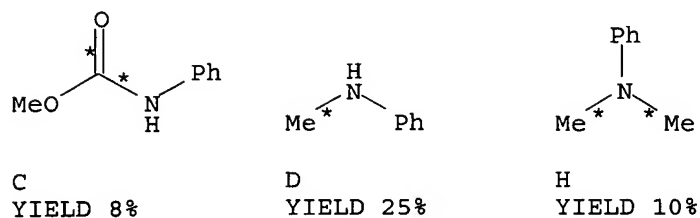
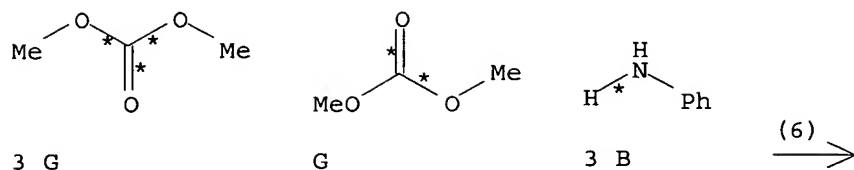
D
YIELD 20%



H
YIELD 2%

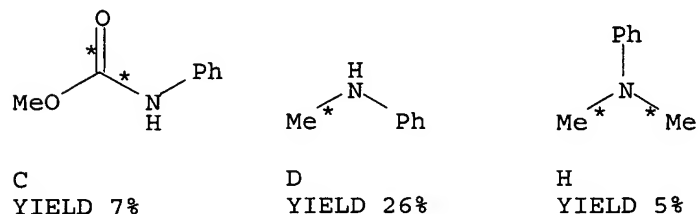
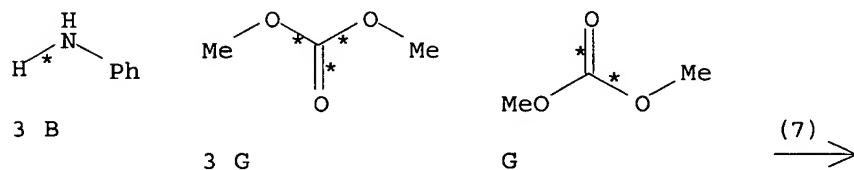
RX(3) RCT B 62-53-3, G 616-38-6
 PRO C 2603-10-3, D 100-61-8, H 121-69-7
 CAT 144026-79-9 Methanesulfonic acid, trifluoro-, scandium(3+) salt
 SOL 109-99-9 THF
 CON 27 hours, 363K

RX(6) OF 12 4 G + 3 B ==> C + D + H



RX(6) RCT G 616-38-6, B 62-53-3
 PRO C 2603-10-3, D 100-61-8, H 121-69-7
 CAT 144026-79-9 Methanesulfonic acid, trifluoro-, scandium(3+) salt
 CON SUBSTAGE(1) 24 hours, 363K
 SUBSTAGE(2) 363K -> room temperature
 NTE no solvent

RX(7) OF 12 3 B + 4 G ==> C + D + H



RX(7) RCT B 62-53-3, G 616-38-6
 PRO C 2603-10-3, D 100-61-8, H 121-69-7
 CAT 52093-26-2 Methanesulfonic acid, trifluoro-, lanthanum(3+) salt
 SOL 109-99-9 THF
 CON 26 hours, 363K

L60 ANSWER 15 OF 44 CASREACT COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 138:137040 CASREACT

TITLE: Process for the production of 1,2,4-triaminobenzene carbamic acid esters by amidation with pyrocarbonate or polypyrocarbonate esters

INVENTOR(S): Lankau, Hans-Joachim; Unverferth, Klaus; Arnold, Thomas; Schaefer, Jorgen; Meisel, Peter; Thiel, Wilfried

PATENT ASSIGNEE(S): Germany

SOURCE: U.S. Pat. Appl. Publ., 6 pp.
CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

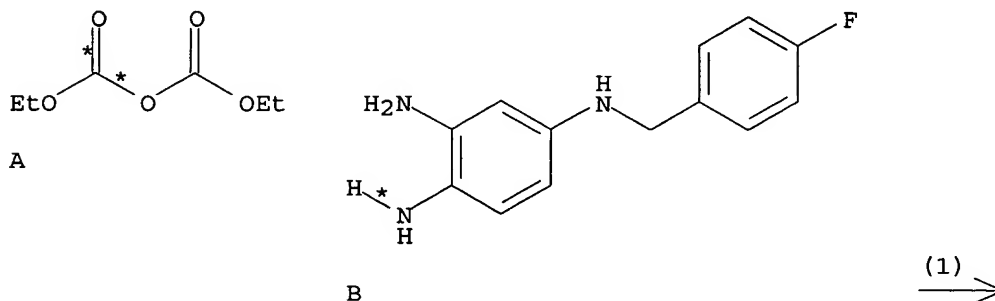
PATENT INFORMATION:

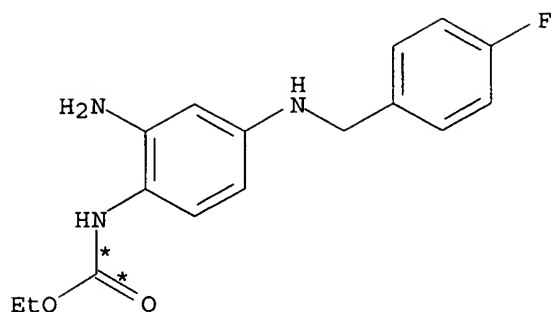
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2003023111	A1	20030130	US 2002-201296	20020724
DE 10136046	A1	20030213	DE 2001-10136046	20010725
WO 2003010134	A1	20030206	WO 2002-EP7301	20020702
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1414791	A1	20040506	EP 2002-790169	20020702
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				
JP 2004536142	T2	20041202	JP 2003-515494	20020702
PRIORITY APPLN. INFO.:			DE 2001-10136046	20010725
			WO 2002-EP7301	20020702

OTHER SOURCE(S): MARPAT 138:137040

AB A process for the production of 1,2,4-triaminobenzene carbamic acid esters is described which is characterized by the use of pyrocarbonate (e.g., Et polypyrocarbonate) or polypyrocarbonate esters. The use of pyrocarbonate or polypyrocarbonate esters brings about a rise in yield and increased purity of the product.

RX(1) OF 1 A + B ==> C





C
YIELD 67%

RX(1) RCT A 1609-47-8, B 491871-67-1
PRO C 150812-12-7
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 2.5 hours, 6 - 11 deg C
SUBSTAGE(2) 3 hours, 6 - 11 deg C
SUBSTAGE(3) 11 deg C -> -5 deg C
SUBSTAGE(4) 2 hours, 5 - -5 deg C
NTE optimization study

L60 ANSWER 16 OF 44 CASREACT COPYRIGHT 2006 ACS on STN

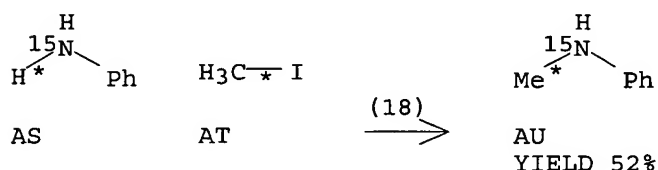
ACCESSION NUMBER: 140:164000 CASREACT
TITLE: Trans Influence on the Rate of Reductive Elimination.
Reductive Elimination of Amines from Isomeric
Arylpalladium Amides with Unsymmetrical Coordination
Spheres
AUTHOR(S): Yamashita, Makoto; Vicario, Jose V. Cuevas; Hartwig,
John F.
CORPORATE SOURCE: Department of Chemistry, Yale University, New Haven,
CT, 06520-8107, USA
SOURCE: Journal of the American Chemical Society (2003),
125(52), 16347-16360
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB To determine the trans effect on the rates of reductive eliminations from arylpalladium(II) amido complexes, the reactions of arylpalladium amido complexes bearing sym. and unsym. DPPF (DPPF = bis(diphenylphosphino)ferrocene) ligands were studied. THF solns. of LPd(Ar) (NMeAr') (L = DPPF, DPPF-OMe, DPPF-CF₃, DPPF-OMe, Ph, DPPF-Ph, CF₃, and DPPF-OMe, CF₃; Ar = C₆H₄-4-CF₃; Ar' = C₆H₄-4-Me, Ph, and C₆H₄-4-OMe) underwent C-N bond forming reductive elimination at -15° to form the corresponding N-methyldiarylamine in high yield. Complexes ligated by sym. DPPF derivs. with electron-withdrawing substituents on the DPPF aryl groups underwent reductive elimination faster than complexes ligated by sym. DPPF derivs. with electron-donating substituents. Studies of arylpalladium amido complexes containing unsym. DPPF ligands revealed several trends. First, the complex with the weaker donor trans to nitrogen and the stronger donor trans to the palladium-bound aryl group underwent reductive elimination faster than the regioisomeric complex with the stronger donor trans to nitrogen and the weaker donor trans to the

palladium-bound aryl group. Second, the substituent effect of the phosphorus donor trans to the nitrogen was larger than the effect of the phosphorus donor trans to the palladium-bound aryl group. Third, the difference in rate between the isomeric arylpalladium amido complexes was similar in magnitude to the differences in rates resulting from conventional variation of substituents on the sym. phosphine ligands. This result suggests that the geometry of the complex is equal in importance to the donating ability of the dative ligands. The ratio of the differences in rates of reaction of the isomeric complexes was similar to the relative populations of the two geometric isomers. This result and consideration of transition state geometries suggest that the reaction rates are controlled more by substituent effects on ground state stability than on transition state energies. In addition, variation of the aryl group at the amido nitrogen showed systematically that complexes with more electron-donating groups at nitrogen undergo faster reductive elimination than those with less electron-donating groups at nitrogen.

REFERENCE COUNT: 111 THERE ARE 111 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(18) OF 88 AS + AT ==> AU...



RX(18) RCT AS 7022-92-6

STAGE(1)

RGT AV 24424-99-5 (Boc)2O
SOL 109-99-9 THF, 7732-18-5 Water
CON 19 hours, room temperature

STAGE(2)

RGT AF 7732-18-5 Water
SOL 7732-18-5 Water

STAGE(3)

RCT AT 74-88-4
RGT AW 7646-69-7 NaH
SOL 68-12-2 DMF
CON 5 hours, room temperature

STAGE(4)

RGT AF 7732-18-5 Water
SOL 7732-18-5 Water

STAGE(5)

RGT AX 1493-13-6 F3CSO2H
SOL 75-09-2 CH2Cl2
CON 1.5 hours, room temperature

STAGE(6)

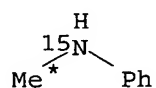
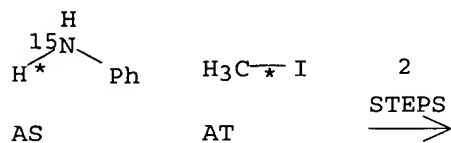
RGT AY 1310-73-2 NaOH

SOL 7732-18-5 Water

PRO AU 60317-46-6

RX(44) OF 88 COMPOSED OF RX(18), RX(19)

RX(44) AS + AT ==> BB



● K

BB

YIELD 44%

RX(18) RCT AS 7022-92-6

STAGE(1)

RGT AV 24424-99-5 (Boc)2O

SOL 109-99-9 THF, 7732-18-5 Water

CON 19 hours, room temperature

STAGE(2)

RGT AF 7732-18-5 Water

SOL 7732-18-5 Water

STAGE(3)

RCT AT 74-88-4

RGT AW 7646-69-7 NaH

SOL 68-12-2 DMF

CON 5 hours, room temperature

STAGE(4)

RGT AF 7732-18-5 Water

SOL 7732-18-5 Water

STAGE(5)

RGT AX 1493-13-6 F3CSO2H

SOL 75-09-2 CH2Cl2

CON 1.5 hours, room temperature

STAGE(6)

RGT AY 1310-73-2 NaOH

SOL 7732-18-5 Water

PRO AU 60317-46-6

RX(19) RCT AU 60317-46-6
 RGT O 40949-94-8 K [N(SiMe₃)₂]
 PRO BB 653588-24-0
 SOL 108-88-3 PhMe
 CON 1 - 1.5 hour, room temperature

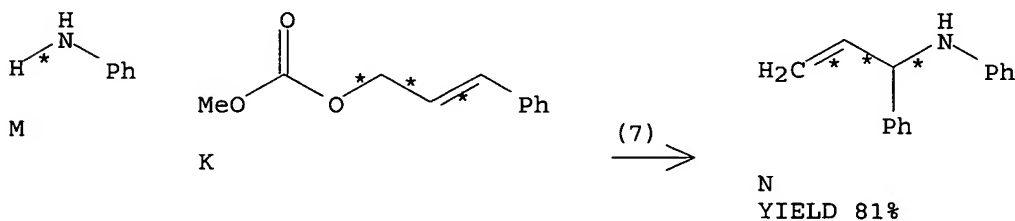
L60 ANSWER 17 OF 44 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 140:59365 CASREACT
 TITLE: Identification of an Activated Catalyst in the Iridium-Catalyzed Allylic Amination and Etherification. Increased Rates, Scope, and Selectivity
 AUTHOR(S): Kiener, Christoph A.; Shu, Chutian; Incarvito, Christopher; Hartwig, John F.
 CORPORATE SOURCE: Department of Chemistry, Yale University, New Haven, CT, 06520-8107, USA
 SOURCE: Journal of the American Chemical Society (2003), 125(47), 14272-14273
 CODEN: JACSAT; ISSN: 0002-7863
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB Studies were conducted to determine possible intermediates in the highly enantioselective, iridium-catalyzed amination and etherification of allylic carbonates, and these studies revealed that cyclometalation of the phosphoramidite ligand is likely to generate the active catalyst. The square-planar [Ir(COD)(L1)Cl] [L1 = (11bS)-N,N-bis[(1S)-1-phenylethyl]dinaphtho[2,1-d:1',2'-f][1,3,2]dioxaphosphepin-4-amine] did not react with cinnamyl carbonate, but did react with amine to generate an Ir(I) trigonal bipyramidal complex coordinated by COD, a cyclometalated κ^2 -phosphoramidite, and a κ^1 -phosphoramidite. This complex reacted with phosphines to generate products from replacement of the κ^1 -phosphoramidite. These cyclometalated complexes were highly active catalysts for allylic amination and etherification and retained the high selectivity of the original catalyst system. In addition, these complexes combined with [Ir(COD)Cl]₂ catalyzed reactions of amines with lower loadings, catalyzed reactions of alkylamines and aromatic amines that did not react with the original catalyst system, and catalyzed reactions of phenoxides under milder conditions.

REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

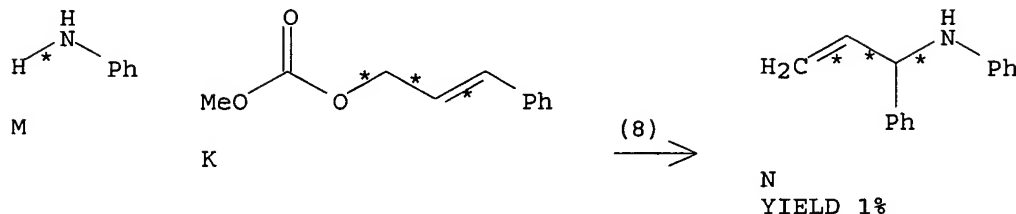
RX(7) OF 18 M + K ==> N



RX(7) RCT M 62-53-3, K 85217-69-2

PRO N 638166-19-5
 CAT 638166-14-0 Iridium, [(11bS)-N,
 , 12112-67-3 Iridium, di- μ -chlorobis[(1,2,5,6- η)-1,5-
 cyclooctadiene]di-
 SOL 109-99-9 THF
 CON 2 hours, 25 deg C
 NTE stereoselective

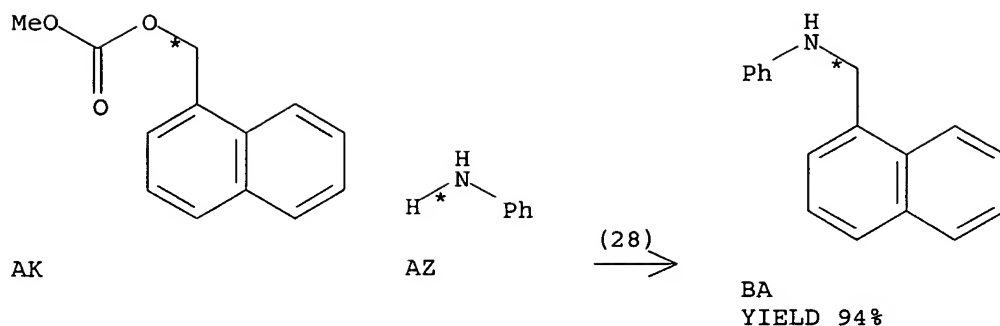
RX(8) OF 18 M + K ==> N



RX(8) RCT M 62-53-3, K 85217-69-2
 PRO N 638166-19-5
 CAT 209482-27-9 Dinaphtho[2,1-d:1',2'-f][1,3,2]dioxaphosphepin-4-
 amine, N,N-bis[(1S)-1-phenylethyl]-, (11bS)-, 12112-67-3
 Iridium, di- μ -chlorobis[(1,2,5,6- η)-1,5-cyclooctadiene]di-
 SOL 109-99-9 THF
 CON 24 hours, 25 deg C
 NTE stereoselective

L60 ANSWER 18 OF 44 CASREACT COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 139:323314 CASREACT
 TITLE: Palladium-Catalyzed Nucleophilic Benzylic
 Substitutions of Benzylic Esters
 AUTHOR(S): Kuwano, Ryoichi; Kondo, Yutaka; Matsuyama, Yosuke
 CORPORATE SOURCE: Department of Chemistry, Graduate School of Sciences,
 Kyushu University, Higashi-ku Fukuoka, 812-8581, Japan
 SOURCE: Journal of the American Chemical Society (2003),
 125(40), 12104-12105
 CODEN: JACSAT; ISSN: 0002-7863
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB A palladium complex generated in situ from [Pd(η^3 -C₃H₅)(cod)]BF₄ and
 DPPF is a good catalyst for benzylic alkylation of benzyl Me carbonate
 with the carbanion of di-Me malonates. The catalytic reaction is
 applicable to a wide range of the benzylations of benzylic esters with
 malonates. The catalytic activity was heavily affected by the bite angle
 of the bidentate phosphine ligand on palladium. DPEphos ligand is superior
 to DPPF in the case of palladium-catalyzed benzylic amination of benzylic
 esters.
 REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(28) OF 28 AK + AZ ==> BA



RX(28) RCT AK 613670-57-8, AZ 62-53-3
 PRO BA 7182-94-7
 CAT 166330-10-5 Phosphine, (oxydi-2,1-phenylene)bis[diphenyl-,
 32915-11-0 Palladium(1+), [(1,2,5,6-η)-1,5-
 cyclooctadiene](η3-2-propenyl)-, tetrafluoroborate(1-)
 SOL 110-71-4 (CH₂OMe)₂
 CON 24 hours, 80 deg C

L60 ANSWER 19 OF 44 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 139:70686 CASREACT

TITLE: Activity of amorphous V-AlPO₄ and Co-AlPO₄ in the
 selective synthesis of N-monoalkylated aniline via
 alkylation of aniline with methanol or dimethyl
 carbonate

AUTHOR(S): Nagaraju, N.; Kuriakose, George

CORPORATE SOURCE: Department of Chemistry, St. Joseph's College Post
 Graduate Center, Bangalore, 560 027, India

SOURCE: New Journal of Chemistry (2003), 27(4), 765-768
 CODEN: NJCHE5; ISSN: 1144-0546

PUBLISHER: Royal Society of Chemistry

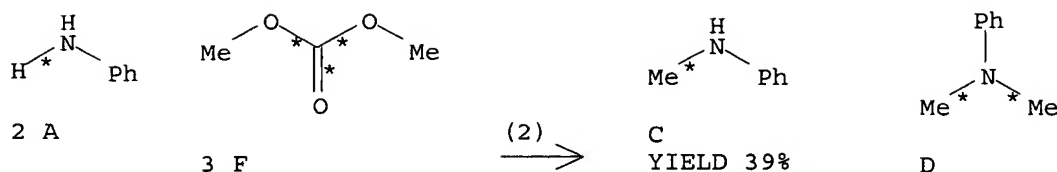
DOCUMENT TYPE: Journal

LANGUAGE: English

AB The vapor phase catalytic alkylation of aniline with methanol or di-Me
 carbonate (DMC) on amorphous AlPO₄ and M-AlPO₄ (M = Cu, Ni, Fe, Co and V)
 as catalysts was studied. Both V-AlPO₄ and Co-AlPO₄ showed high
 selectivity towards N-monomethylation of aniline. Further studies on the
 alkylation reactions were carried out using AlPO₄ and M-AlPO₄ (M = V and
 Co) as catalysts at different temps. and molar ratio of aniline to
 methanol or DMC. V-AlPO₄ showed 100% selectivity for N-monomethylation of
 aniline, irres. of the temperature or the molar ratio of the reactants.
 Co-AlPO₄ showed 100% selectivity for N-monomethylated product only when
 the aniline-to-methanol (or DMC) molar ratio is 2:1. The aniline
 conversion towards N-methylaniline (NMA) was 39%. DMC was a better
 methylating agent than methanol with respect to the percentage conversion
 of aniline to N-methylaniline.

REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

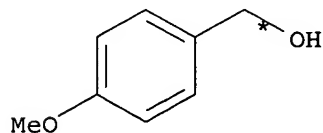
RX(2) OF 2 2 A + 3 F ==> C + D



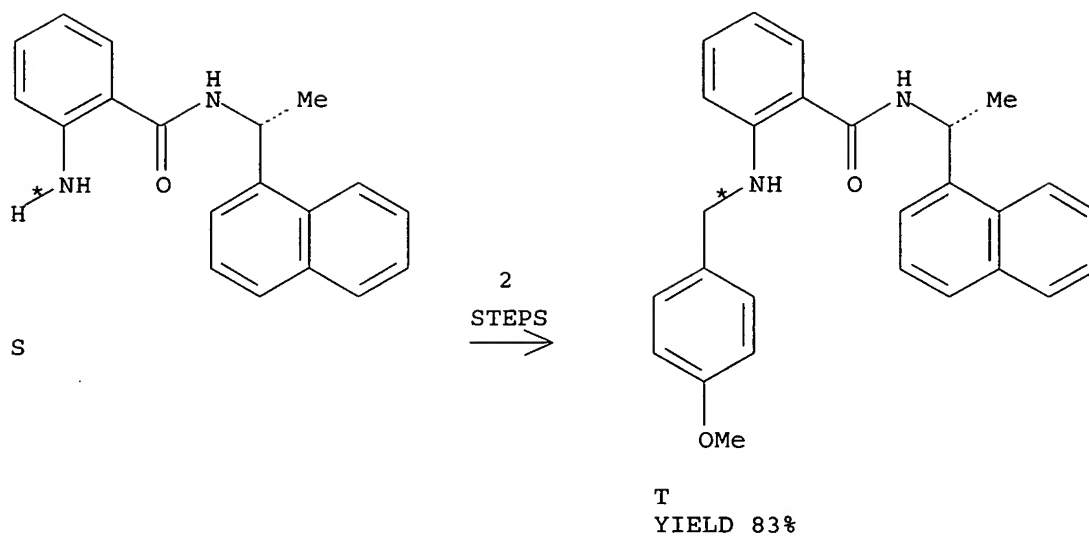
RX(2) RCT A 62-53-3, F 616-38-6
 PRO C 100-61-8, D 121-69-7
 CAT 501936-33-0 Phosphoric acid, aluminum vanadium salt
 CON 523K
 NTE gas phase, down-flow fixed-bed glass reactor used, yield depends
 on reaction conditions, thermal

L60 ANSWER 20 OF 44 CASREACT COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 141:190769 CASREACT
 TITLE: Intrinsic sensing fluorescent probe for the solid
 phase synthesis of 1,4-benzodiazepine-2,5-dione
 AUTHOR(S): Rivero, Ignacio A.; Peralta, Margarita; Heredia,
 Socorro; Madrigal, Domingo; Pina-Luis, Georgina;
 Chavez, Daniel
 CORPORATE SOURCE: Centro de Graduados e Investigacion, Instituto
 Tecnologico de Tijuana, Tijuana, 22000, Mex.
 SOURCE: ARKIVOC (Gainesville, FL, United States) (2003), (11),
 27-36
 CODEN: AGFUAR
 URL: http://www.arkat-usa.org/ark/journal/2003/Regional_Issue/MX-827E/827E.pdf
 PUBLISHER: Arkat USA Inc.
 DOCUMENT TYPE: Journal; (online computer file)
 LANGUAGE: English
 AB The synthesis of 4-N-naphthylethyl-1,4-benzodiazepine-2,5-dione supported
 on solid phase is described. The fluorescent naphthyl group is used as
 internal sensor for monitoring various stages on the synthetic reaction by
 spectral differences in fluorescence. Our results show the efficacy of
 fluorescence as a direct method for the evaluation of reaction progress.
 This method is fast, sensitive and non-destructive. A target mol. was
 synthesized which could be used in the synthesis of a variety of
 benzodiazepines.
 REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(60) OF 162 COMPOSED OF RX(7), RX(8)
 RX(60) Q + S ==> T



Q



RX(7) RCT Q 105-13-5D

STAGE(1)

SOL 75-09-2 CH₂Cl₂

CON 30 minutes, room temperature

STAGE(2)

RGT L 603-35-0 PPh₃

SOL 75-09-2 CH₂Cl₂

CON 5 minutes, 0 deg C

STAGE(3)

RGT M 32315-10-9 (Cl₃CO)₂CO

CON 5 minutes, 0 deg C

STAGE(4)

SOL 75-09-2 CH₂Cl₂

CON room temperature

STAGE(5)

SOL 75-09-2 CH₂Cl₂

CON 1 hour, room temperature

PRO R 824-94-2D

NTE solid-supported reaction, crude from stage 2,3 added in stage 4

RX(8) RCT R 824-94-2D

STAGE(1)

SOL 68-12-2 DMF

CON 30 minutes, room temperature

STAGE(2)

RCT S 737765-26-3

RGT U 584-08-7 K₂CO₃

CON SUBSTAGE(1) room temperature

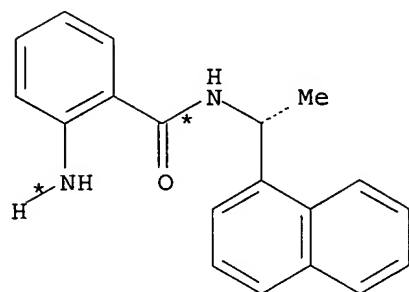
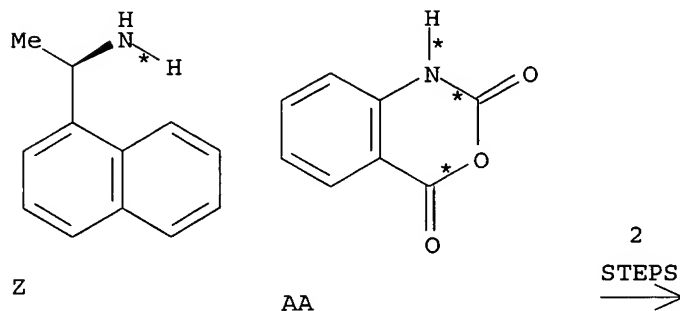
SUBSTAGE(2) 12 hours, 80 deg C

PRO T 737765-27-4D
NTE solid-supported reaction

RX(97) OF 162 COMPOSED OF REACTION SEQUENCE RX(16), RX(8)
AND REACTION SEQUENCE RX(7), RX(8)

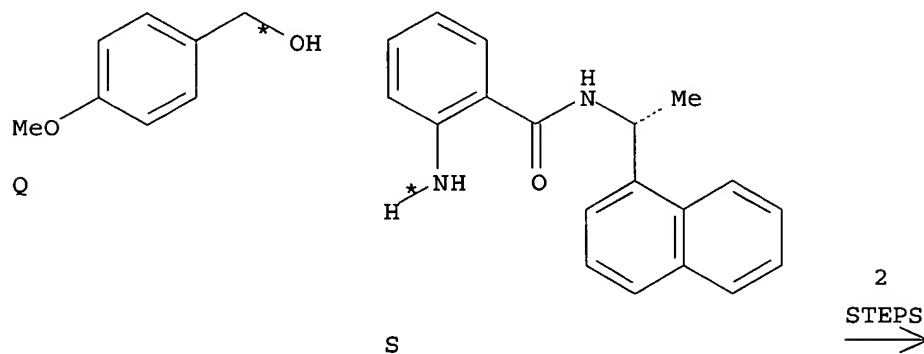
...Z + AA ==> S...

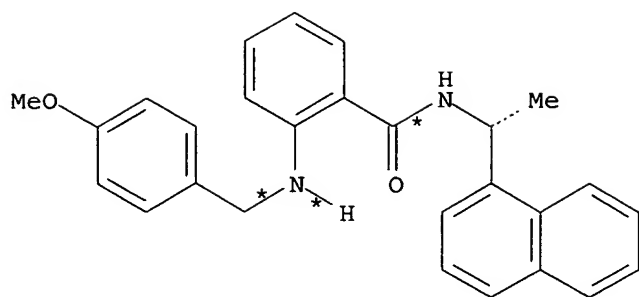
...Q + S ==> T



S

START NEXT REACTION SEQUENCE





T
YIELD 83%

RX(16) RCT Z 3886-70-2, AA 118-48-9

STAGE(1)

SOL 68-12-2 DMF

CON SUBSTAGE(1) 20 minutes, 55 deg C

SUBSTAGE(2) 2 hours, 55 - 60 deg C

STAGE(2)

SOL 7732-18-5 Water

PRO S 737765-26-3

RX(7) RCT Q 105-13-5D

STAGE(1)

SOL 75-09-2 CH₂Cl₂

CON 30 minutes, room temperature

STAGE(2)

RGT L 603-35-0 PPh₃

SOL 75-09-2 CH₂Cl₂

CON 5 minutes, 0 deg C

STAGE(3)

RGT M 32315-10-9 (Cl₃CO)₂CO

CON 5 minutes, 0 deg C

STAGE(4)

SOL 75-09-2 CH₂Cl₂

CON room temperature

STAGE(5)

SOL 75-09-2 CH₂Cl₂

CON 1 hour, room temperature

PRO R 824-94-2D

NTE solid-supported reaction, crude from stage 2,3 added in stage 4

RX(8) RCT R 824-94-2D

STAGE(1)

SOL 68-12-2 DMF

CON 30 minutes, room temperature

STAGE(2)

RCT S 737765-26-3

RGT U 584-08-7 K2CO3

CON SUBSTAGE(1) room temperature

SUBSTAGE(2) 12 hours, 80 deg C

PRO T 737765-27-4D

NTE solid-supported reaction

L60 ANSWER 21 OF 44 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 139:373878 CASREACT

TITLE: Molecular design and biological activities of protein-tyrosine phosphatase inhibitors

AUTHOR(S): Umezawa, Kazuo; Kawakami, Mariko; Watanabe, Takumi

CORPORATE SOURCE: Faculty of Science and Technology, Department of Applied Chemistry, Keio University, Kohoku-ku, Yokohama, 223-0061, Japan

SOURCE: Pharmacology & Therapeutics (2003), 99(1), 15-24

CODEN: PHTHDT; ISSN: 0163-7258

PUBLISHER: Elsevier Science B.V.

DOCUMENT TYPE: Journal; General Review

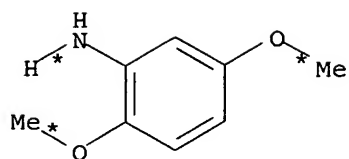
LANGUAGE: English

AB A review. Protein-tyrosine kinase (PTKase) and protein-tyrosine phosphatase (PTPase) regulate the intracellular signal transduction in various biol. processes. PTPase often neg. regulates the intracellular protein-tyrosine phosphorylation. PTPases are considered to be involved in the etiol. of diabetes mellitus and neural diseases, such as Alzheimer's disease and Parkinson's disease. Therefore, PTPase inhibitors should be useful tools to study the role of PTPases in these diseases and other biol. phenomena, and they hopefully may be developed into chemotherapeutic agents. We first discovered a naturally occurring PTPase inhibitor, dephostatin, in 1993. Later, we developed stable and safe dephostatin analogs by a mol. design approach employing the concept of CH/ π interaction. We prepared Et-3,4-dephostatin as a stable analog and found it to inhibit PTP-1B and SHPTP-1 PTPases selectively. Et-3,4-dephostatin increased the tyrosine phosphorylation of the insulin receptor and insulin receptor substrate-1 (IRS-1), with or without insulin, in differentiated 3T3-L1 mouse adipocytes. It also increased the phosphorylation and activation of Akt. The analog also enhanced translocation of glucose transporter 4 (GLUT4) from the cytoplasm to the membrane and 2-deoxyglucose transport. It also showed an in vivo antidiabetic effect in terms of reducing the high blood glucose level in KK-Ay mice after oral administration. Since Et-3,4-dephostatin contains a nitrosamine moiety, we designed nitrosamine-free dephostatin analogs employing the concept of CH/ π interaction. Then, we synthesized methoxime- and hexyl-methoxime-3,4-dephostatin as nitrosamine-free analogs. These analogs also showed antidiabetic activity in vivo and illustrate the utility of the CH/ π interaction mol. design approach.

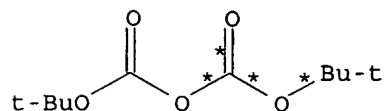
REFERENCE COUNT: 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(19) OF 26 COMPOSED OF RX(1), RX(2), RX(3)

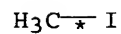
RX(19) A + B + G ==> K



A

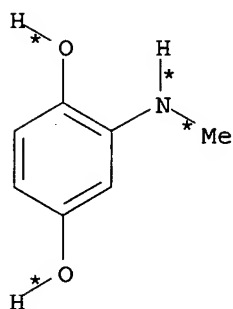


B



G

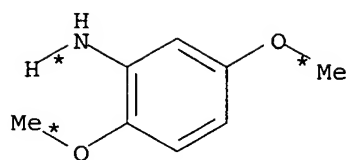
3
STEPS
→



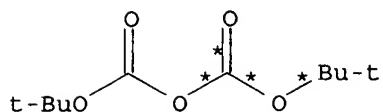
K

RX(1)	RCT	A 102-56-7, B 24424-99-5
	RGT	D 121-44-8 Et3N
	PRO	C 170959-02-1
	SOL	7732-18-5 Water, 123-91-1 Dioxane
RX(2)	RCT	C 170959-02-1, G 74-88-4
	RGT	I 7646-69-7 NaH
	PRO	H 155853-12-6
	SOL	68-12-2 DMF
RX(3)	RCT	H 155853-12-6
	RGT	L 10294-33-4 BBr3
	PRO	K 155853-13-7
	SOL	75-09-2 CH2Cl2

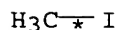
RX(20) OF 26 COMPOSED OF RX(1), RX(2), RX(11)
 RX(20) A + B + G + 2 AJ ==> N



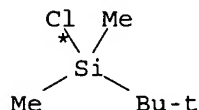
A



B

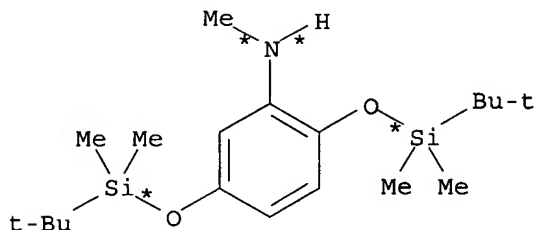


G



2 AJ

3
STEPS
→



N
YIELD 41%

RX(1) RCT A 102-56-7, B 24424-99-5
RGT D 121-44-8 Et3N
PRO C 170959-02-1
SOL 7732-18-5 Water, 123-91-1 Dioxane

RX(2) RCT C 170959-02-1, G 74-88-4
RGT I 7646-69-7 NaH
PRO H 155853-12-6
SOL 68-12-2 DMF

RX(11) RCT H 155853-12-6

STAGE(1)

RGT L 10294-33-4 BBr3
SOL 75-09-2 CH2Cl2

STAGE(2)

RCT AJ 18162-48-6
RGT AK 288-32-4 1H-Imidazole
SOL 68-12-2 DMF

PRO N 155853-14-8

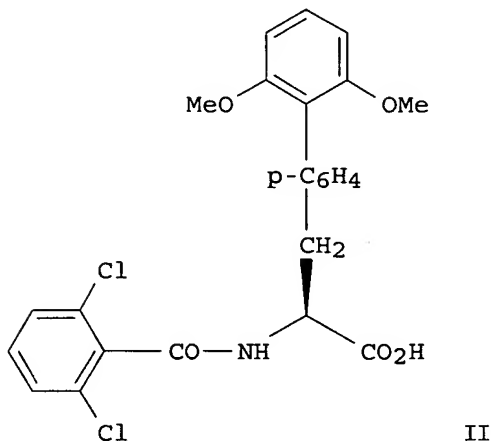
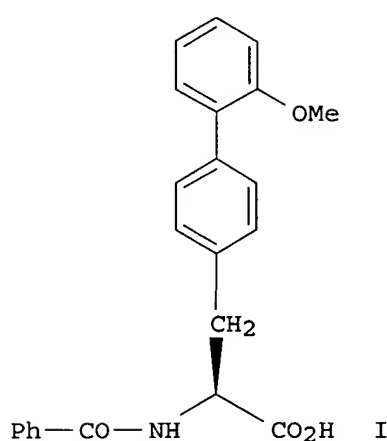
L60 ANSWER 22 OF 44 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 137:263272 CASREACT

TITLE: Synthesis and SAR of N-Benzoyl-L-Biphenylalanine
Derivatives: Discovery of TR-14035, A Dual
 $\alpha 4\beta 7/\alpha 4\beta 1$ Integrin Antagonist

AUTHOR(S): Sircar, Ila; Gudmundsson, Kristjan S.; Martin,
Richard; Liang, Jimmy; Nomura, Sumihiro; Jayakumar,
Honnappa; Teegarden, Bradley R.; Nowlin, Dawn M.;
Cardarelli, Pina M.; Mah, Jason R.; Connell, Samuel;
Griffith, Ronald C.; Lazarides, Elias

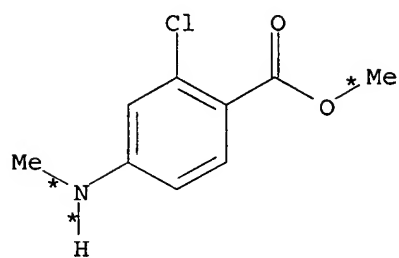
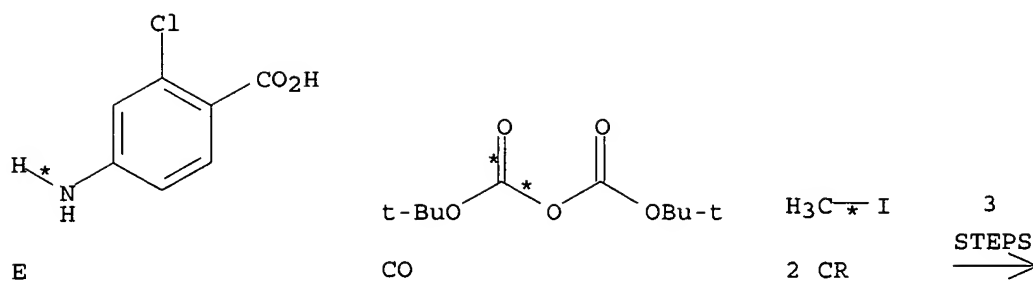
CORPORATE SOURCE: Department of Chemical Science, Tanabe Research
Laboratories USA, Inc., San Diego, CA, 92121, USA
SOURCE: Bioorganic & Medicinal Chemistry (2002), 10(6),
2051-2066
CODEN: BMECEP; ISSN: 0968-0896
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



AB $\alpha 4\beta 1$ And $\alpha 4\beta 7$ integrins are key regulators of
physiol. and pathol. responses in inflammation and autoimmune disease.
The effectiveness of anti-integrin antibodies to attenuate a number of
inflammatory/immune conditions provides a strong rationale to target
integrins for drug development. Important advances have been made in
identifying potent and selective candidates, peptides and peptidomimetics,
for further development. Herein, we report the discovery of a series of
novel N-benzoyl-L-biphenylalanine derivs. that are potent inhibitors of
 $\alpha 4$ integrins. The potency of the initial lead compound (I: IC₅₀
 $\alpha 4\beta 7/\alpha 4\beta 1=5/33 \mu\text{M}$) was optimized via sequential
manipulation of substituents to generate low nM, orally bioavailable dual
 $\alpha 4\beta 1/\alpha 4\beta 7$ antagonists. The SAR also led to the
identification of several subnanomolar antagonists. Compound (II)
(TR-14035; IC₅₀ $\alpha 4\beta 7/\alpha 4\beta 1=7/87 \text{ nM}$) has completed
Phase I studies in Europe. The synthesis, SAR and biol. evaluation of
these compds. are described.

REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(224) OF 267 COMPOSED OF RX(42), RX(43), RX(4)
RX(224) E + CO + 2 CR ==> Q



Q

RX (42) RCT E **2457-76-3**, CO **24424-99-5**
 RGT DJ 1310-73-2 NaOH
 PRO DO 232275-73-9
 SOL 123-91-1 Dioxane

RX (43) RCT DO 232275-73-9

STAGE (1)

RGT DP 124-41-4 NaOMe
SOL 68-12-2 DMF

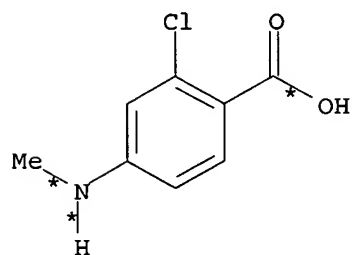
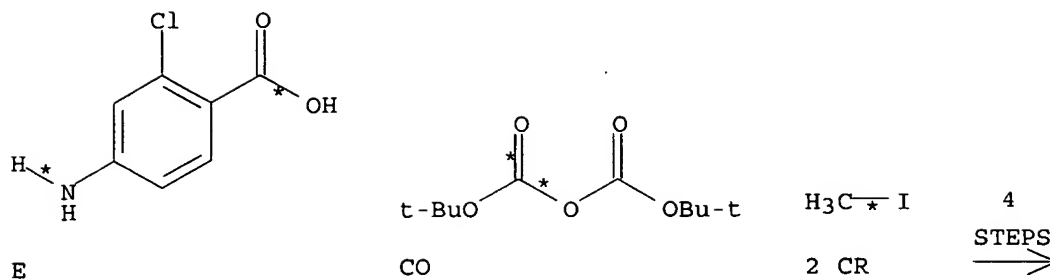
STAGE (2)

RCT CR 74-88-4

PRO P 232275-74-0

RX (4) RCT P 232275-74-0
 RGT B 76-05-1 F3CCO2H
 PRO Q **204972-82-7**
 SOL 75-09-2 CH2Cl2

RX(227) OF 267 COMPOSED OF RX(42), RX(43), RX(4), RX(44)
 RX(227) E + CO + 2 CR ==> DQ



DQ

RX(42) RCT E 2457-76-3, CO 24424-99-5
 RGT DJ 1310-73-2 NaOH
 PRO DO 232275-73-9
 SOL 123-91-1 Dioxane

RX(43) RCT DO 232275-73-9

STAGE(1)

RGT DP 124-41-4 NaOMe
 SOL 68-12-2 DMF

STAGE(2)

RCT CR 74-88-4

PRO P 232275-74-0

RX(4) RCT P 232275-74-0
 RGT B 76-05-1 F3CCO2H
 PRO Q 204972-82-7
 SOL 75-09-2 CH2Cl2

RX(44) RCT Q 204972-82-7
 RGT AV 1310-65-2 LiOH
 PRO DQ 3975-62-0
 SOL 109-99-9 THF, 67-56-1 MeOH

✓ L60 ANSWER 23 OF 44 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 138:237878 CASREACT

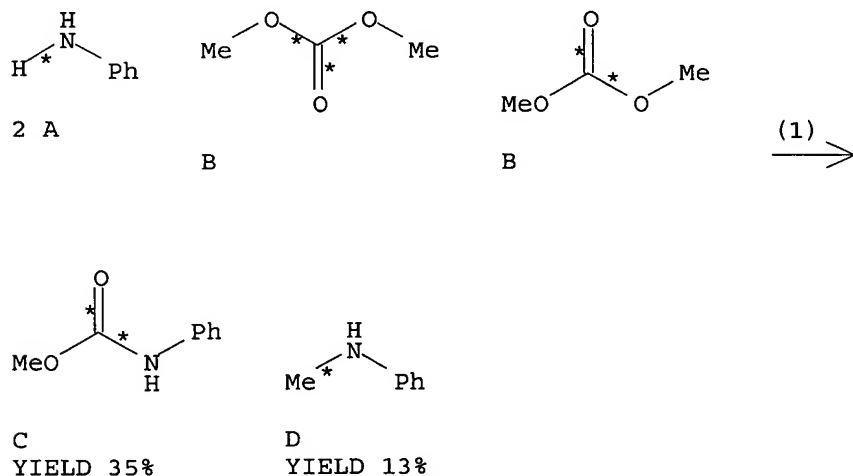
TITLE: A new catalyst for the synthesis of N,N-biphenylurea
 from aniline and dimethyl carbonate

AUTHOR(S): Nagaraju, N.; Kuriakose, George
 CORPORATE SOURCE: Department of Chemistry, St. Joseph's College Post
 Graduate Center, Shanthi Nagar, Bangalore, 560 027,
 India
 SOURCE: Green Chemistry (2002), 4(3), 269-271
 CODEN: GRCHFJ; ISSN: 1463-9262
 PUBLISHER: Royal Society of Chemistry
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB An environmentally benign method for the synthesis of biphenylurea (BPU) in the presence of ecofriendly catalysts was reported. Catalytic activity of various metal aluminophosphates, M-AlPO₄ (M = V, Fe, Co, Ni and Cu) and cobalt supported on hydrated Al₂O₃, SiO₂ and ZrO₂ was studied in the synthesis of BPU from aniline and di-Me carbonate (DMC). All the catalysts used are amorphous. The catalytic activity studies were carried out in the liquid phase under refluxing conditions. Formation of BPU is found to depend on the type of the catalyst, the molar ratio of aniline to DMC and the duration of the reaction. N-Methylaniline and Me N-phenylcarbamate are formed as byproducts of the reaction. Of all the catalysts used, Co-AlPO₄ was found to yield the highest percentage of BPU whereas cobalt supported hydrated Al₂O₃, SiO₂ and ZrO₂ failed to give any BPU.

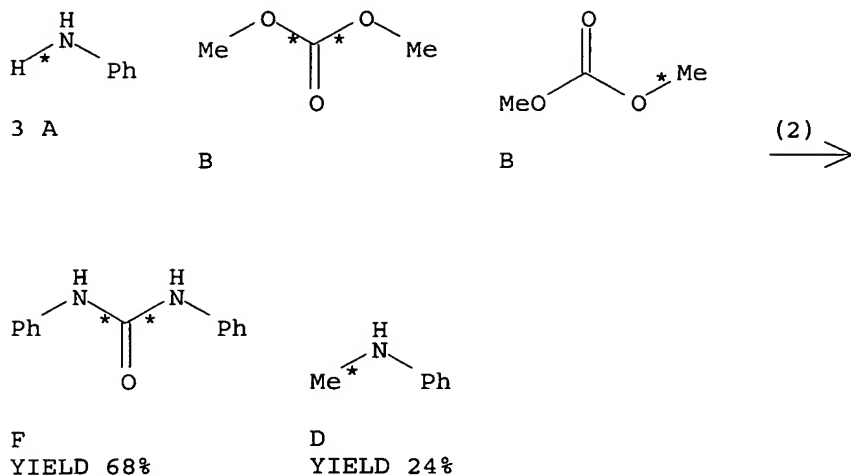
REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(1) OF 2 2 A + 2 B ==> C + D



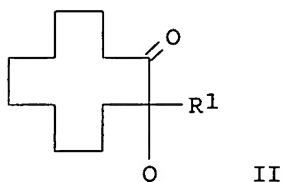
RX(1) RCT A 62-53-3, B 616-38-6
 PRO C 2603-10-3, D 100-61-8
 CAT 23209-38-3 Phosphoric acid, aluminum cobalt salt
 CON 4 hours, reflux
 NTE green chem.-waste redn., optimization study

RX(2) OF 2 3 A + 2 B ==> F + D



RX(2) RCT A 62-53-3, B 616-38-6
 PRO F 102-07-8, D 100-61-8
 CAT 23209-38-3 Phosphoric acid, aluminum cobalt salt
 CON 4 hours, reflux
 NTE green chem.-waste redn., optimization study

L60 ANSWER 24 OF 44 CASREACT COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 137:46974 CASREACT
 TITLE: Synthesis and biological activity of
 2-arylaminomethyl-2-ethoxycarbonylcyclododecanone
 AUTHOR(S): Qi, Chuan-min; Zhang, Guan-xin; Wang, Yun-feng
 CORPORATE SOURCE: Department of Chemistry, Beijing Normal University,
 Beijing, 100875, Peop. Rep. China
 SOURCE: Yingyong Huaxue (2002), 19(3), 243-246
 CODEN: YIHUED; ISSN: 1000-0518
 PUBLISHER: Yingyong Huaxue Bianji Weiyuanhui
 DOCUMENT TYPE: Journal
 LANGUAGE: Chinese
 GI

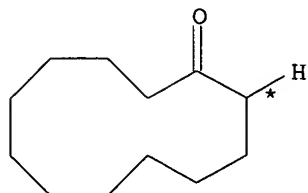


AB Eight title Mannich bases I (R = H, 4-Cl, 2-Cl, 4-CH₃O, 2-Br, 4-Br, 4-CH₃; R₁ = COOCH₂CH₃; Q = CH₂Q₁; Q₁ = NHC₆H₄R) were synthesized from reaction of formaldehyde and dimethylamine hydrochloride and Q₁H with I (Q = CH₂N(CH₃)₂·HCl; R₁ = COOCH₂CH₃), which was prepared from I (R₁ = H; Q = H). Their structures were confirmed by IR, ¹H NMR and elemental anal. Mannich reaction of an amine was occurred at ortho position of 2-ethoxycarbonyl-cyclododecanone. The preliminary in vitro bioassays of

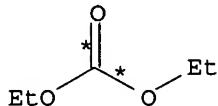
some compds. indicated that some of compds. IV showed certain fungistatic activity against plant pathogens. 4-Br substituted Ph aminomethyl-2-ethoxycarbonyl-cyclododecanone exerted appreciable inhibitory effect on xylene-induced ear edema in mice.

RX(11) OF 17 COMPOSED OF RX(1), RX(3)

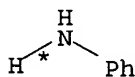
RX(11) A + B + L + G ==> M



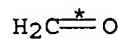
A



B

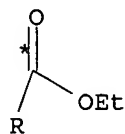
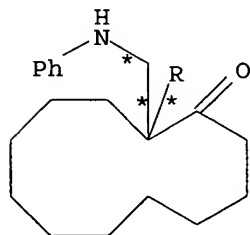


L



G

2
STEPS
→

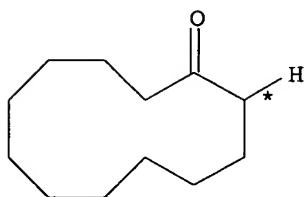


M
YIELD 57%

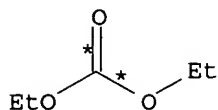
RX(1) RCT A 830-13-7, B 105-58-8
RGT D 7646-69-7 NaH
PRO C 4017-60-1
SOL 71-43-2 Benzene
NTE reflux, 6 h

RX(3) RCT C 4017-60-1, L 62-53-3, G 50-00-0
PRO M 438051-08-2
SOL 64-17-5 EtOH
NTE 50°, 9 h

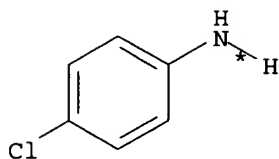
RX(12) OF 17 COMPOSED OF RX(1), RX(4)
 RX(12) A + B + N + G ==> O



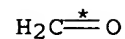
A



B

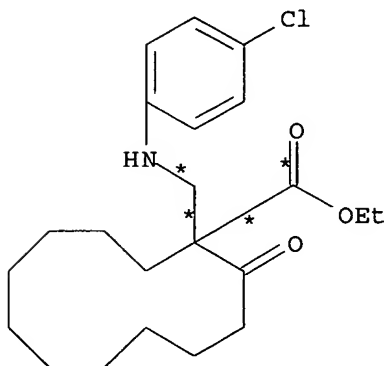


N



G

2
 STEPS
 →

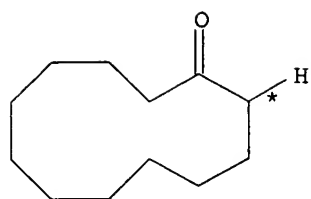


O
 YIELD 49%

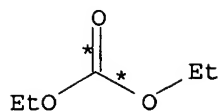
RX(1) RCT A 830-13-7, B 105-58-8
 RGT D 7646-69-7 NaH
 PRO C 4017-60-1
 SOL 71-43-2 Benzene
 NTE reflux, 6 h

RX(4) RCT N 106-47-8, C 4017-60-1, G 50-00-0
 PRO O 438051-10-6
 SOL 64-17-5 EtOH
 NTE room temp.

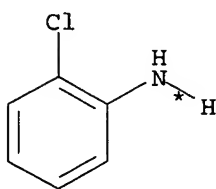
RX(13) OF 17 COMPOSED OF RX(1), RX(5)
 RX(13) A + B + P + G ==> Q



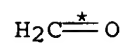
A



B

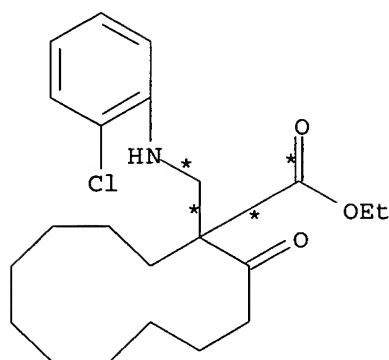


P



G

2
STEPS
→

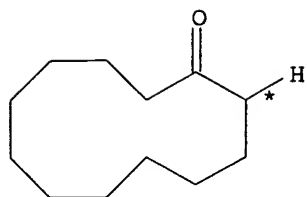


Q
YIELD 42%

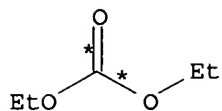
RX(1) RCT A 830-13-7, B 105-58-8
 RGT D 7646-69-7 NaH
 PRO C 4017-60-1
 SOL 71-43-2 Benzene
 NTE reflux, 6 h

RX(5) RCT P 95-51-2, C 4017-60-1, G 50-00-0
 PRO Q 438051-12-8
 SOL 64-17-5 EtOH
 NTE room temp.

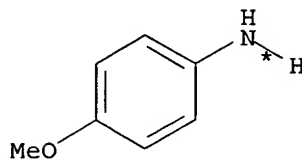
RX(14) OF 17 COMPOSED OF RX(1), RX(6)
 RX(14) A + B + R + G ==> S



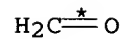
A



B

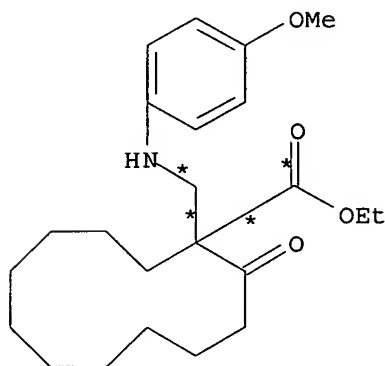


R



G

2
STEPS
→

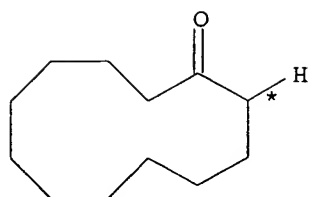


S
YIELD 65%

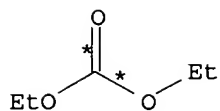
RX(1) RCT A 830-13-7, B 105-58-8
RGT D 7646-69-7 NaH
PRO C 4017-60-1
SOL 71-43-2 Benzene
NTE reflux, 6 h

RX(6) RCT R 104-94-9, C 4017-60-1, G 50-00-0
PRO S 438051-13-9
SOL 64-17-5 EtOH
NTE room temp.

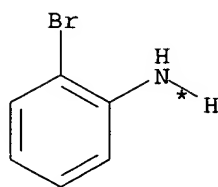
RX(15) OF 17 COMPOSED OF RX(1), RX(7)
RX(15) A + B + T + G ==> U



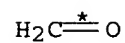
A



B

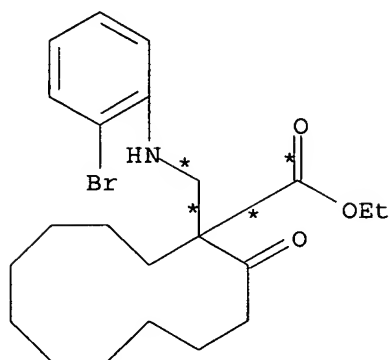


T



G

2
STEPS
→



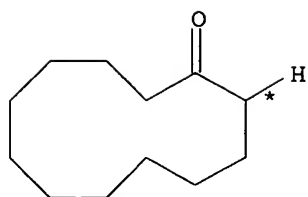
U

YIELD 43%

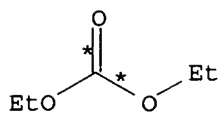
RX(1) RCT A 830-13-7, B 105-58-8
RGT D 7646-69-7 NaH
PRO C 4017-60-1
SOL 71-43-2 Benzene
NTE reflux, 6 h

RX(7) RCT T 615-36-1, C 4017-60-1, G 50-00-0
PRO U 438051-14-0
SOL 64-17-5 EtOH
NTE room temp.

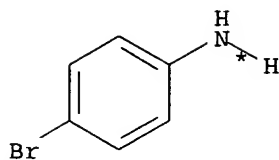
RX(16) OF 17 COMPOSED OF RX(1), RX(8)
RX(16) A + B + V + G ==> W



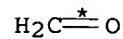
A



B

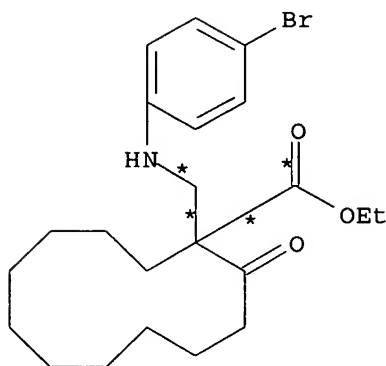


V



G

2
STEPS
→

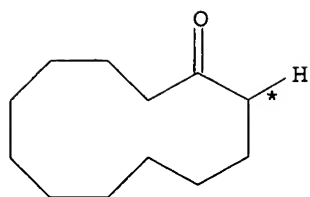


W
YIELD 50%

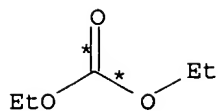
RX(1) RCT A 830-13-7, B 105-58-8
RGT D 7646-69-7 NaH
PRO C 4017-60-1
SOL 71-43-2 Benzene
NTE reflux, 6 h

RX(8) RCT V 106-40-1, C 4017-60-1, G 50-00-0
PRO W 438051-15-1
SOL 64-17-5 EtOH
NTE room temp.

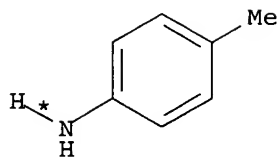
RX(17) OF 17 COMPOSED OF RX(1), RX(9)
RX(17) A + B + X + G ==> Y



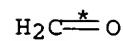
A



B

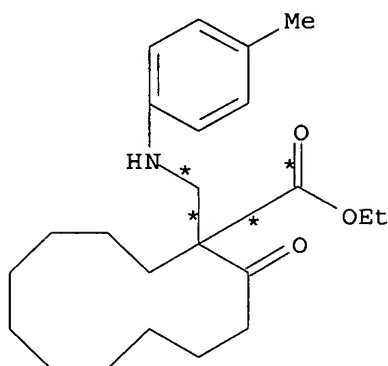


X



G

2
STEPS
→



Y
YIELD 62%

RX(1) RCT A 830-13-7, B 105-58-8
RGT D 7646-69-7 NaH
PRO C 4017-60-1
SOL 71-43-2 Benzene
NTE reflux, 6 h

RX(9) RCT X 106-49-0, C 4017-60-1, G 50-00-0
PRO Y 438051-17-3
SOL 64-17-5 EtOH
NTE room temp.

L60 ANSWER 25 OF 44 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 136:167326 CASREACT

TITLE: Design and Synthesis of Potent Nonpeptidic
Farnesyltransferase Inhibitors Based on a Terphenyl
Scaffold

AUTHOR(S): Ohkanda, Junko; Lockman, Jeffrey W.; Kothare, Mohit
A.; Qian, Yimin; Blaskovich, Michelle A.; Sebt, Said
M.; Hamilton, Andrew D.

CORPORATE SOURCE: Department of Chemistry, Yale University, New Haven,
CT, 06520-8107, USA

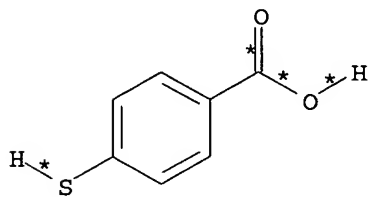
SOURCE: Journal of Medicinal Chemistry (2002), 45(1), 177-188
 CODEN: JMCMAR; ISSN: 0022-2623
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB By modification of key carboxylate, hydrophobic, and zinc-binding groups projected from a sterically restricted terphenyl scaffold, a series of simple and nonpeptide mimetics of the Cys-Val-Ile-Met tetrapeptide substrate of protein farnesyltransferase (FTase) have been designed and synthesized. A crystal structure of 4-nitro-2-phenyl-3'-methoxycarbonylbiphenyl shows that the terphenyl fragment provides a large hydrophobic surface that potentially mimics the hydrophobic side chains of the three terminal residues in the tetrapeptide. 2-Phenyl-3-{N-[1-(4-cyanobenzyl)-1H-imidazol-5-yl]methyl}amino-3'-carboxylbiphenyl, in which the free thiol group was replaced with a 1-(4-cyanobenzyl)imidazole group, shows submicromolar inhibition activity against FTase in vitro and inhibits H-Ras processing in whole cells.

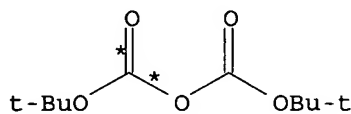
REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(189) OF 350 COMPOSED OF RX(30), RX(31), RX(32), RX(33)

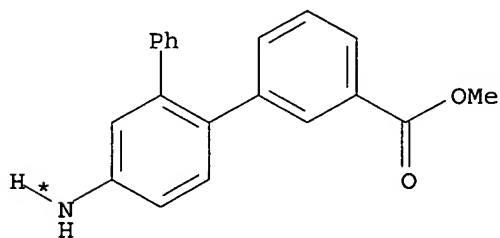
RX(189) CE + CF + AQ ==> BK



CE

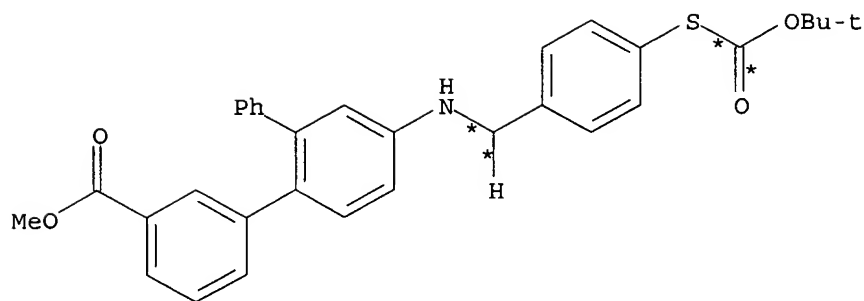


CF



AQ

4
STEPS
→



BK
YIELD 78%

RX(30) RCT CE 1074-36-8, CF **24424-99-5**
 RGT CA 121-44-8 Et3N
 PRO CG 396725-66-9
 CAT 1122-58-3 4-DMAP
 SOL 109-99-9 THF

RX(31) RCT CG 396725-66-9

STAGE(1)
 RGT CA 121-44-8 Et3N, CJ 541-41-3 ClCO2Et
 SOL 109-99-9 THF

STAGE(2)
 RGT CK 16940-66-2 NaBH4

STAGE(3)
 RGT O 7647-01-0 HCl
 SOL 7732-18-5 Water

PRO CI 396725-67-0

RX(32) RCT CI 396725-67-0

STAGE(1)
 RGT CM 79-37-8 (COCl)2, CN 67-68-5 DMSO
 SOL 75-09-2 CH2Cl2

STAGE(2)
 RGT CA 121-44-8 Et3N

PRO CL 396725-68-1

RX(33) RCT CL 396725-68-1, AQ **396725-50-1**

STAGE(1)
 CAT 64-19-7 AcOH
 SOL 75-09-2 CH2Cl2

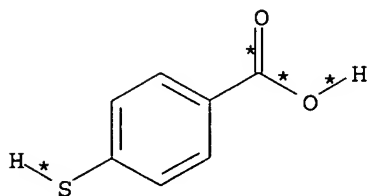
STAGE(2)
 RGT CK 16940-66-2 NaBH4

PRO BK **396725-69-2**

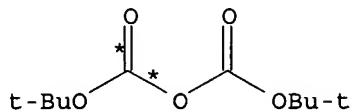
NTE in-situ generated reactant

RX(190) OF 350 COMPOSED OF RX(30), RX(31), RX(32), RX(34)

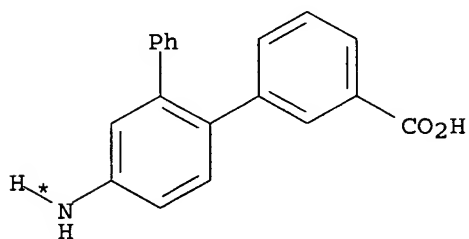
RX(190) CE + CF + AT ==> BH



CE

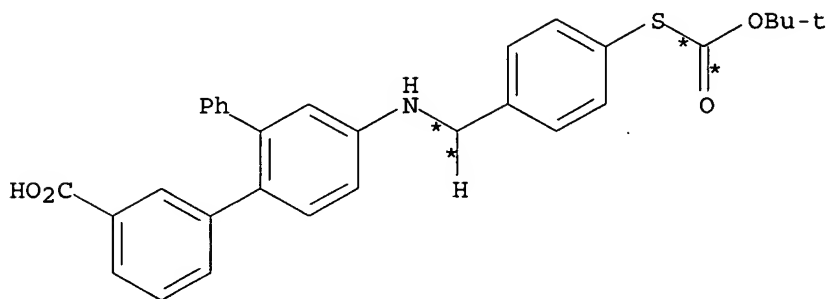


CF



AT

4
STEPS
→



BH
YIELD 23%

RX(30) RCT CE 1074-36-8, CF 24424-99-5
RGT CA 121-44-8 Et3N
PRO CG 396725-66-9
CAT 1122-58-3 4-DMAP
SOL 109-99-9 THF

RX(31) RCT CG 396725-66-9

STAGE(1)

RGT CA 121-44-8 Et3N, CJ 541-41-3 ClCO2Et

SOL 109-99-9 THF

STAGE(2)

RGT CK 16940-66-2 NaBH4

STAGE(3)

RGT O 7647-01-0 HCl

SOL 7732-18-5 Water

PRO CI 396725-67-0

RX(32) RCT CI 396725-67-0

STAGE(1)

RGT CM 79-37-8 (COCl)₂, CN 67-68-5 DMSO

SOL 75-09-2 CH₂Cl₂

STAGE(2)

RGT CA 121-44-8 Et₃N

PRO CL 396725-68-1

RX(34) RCT CL 396725-68-1, AT 191103-10-3

STAGE(1)

CAT 64-19-7 AcOH

SOL 75-09-2 CH₂Cl₂

STAGE(2)

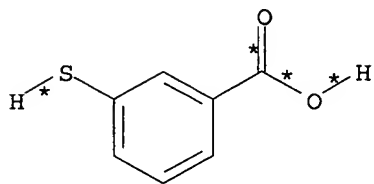
RGT CK 16940-66-2 NaBH₄

PRO BH 396725-70-5

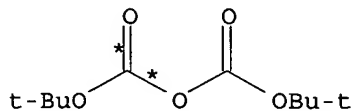
NTE in-situ generated reactant

RX(202) OF 350 COMPOSED OF RX(35), RX(36), RX(37), RX(38)

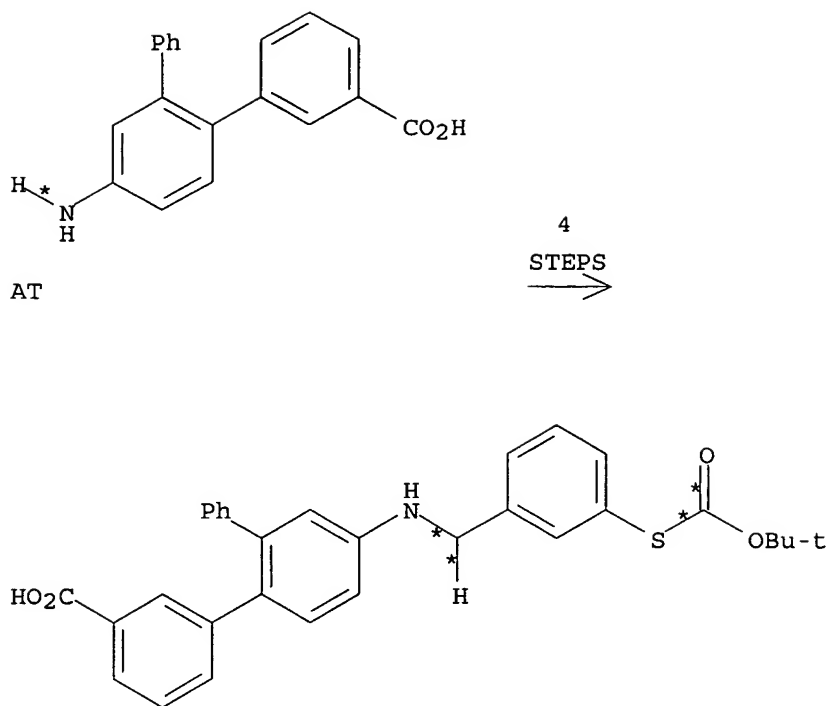
RX(202) CO + CF + AT ==> BM



CO



CF



BM
YIELD 4%

RX(35) RCT CO 4869-59-4, CF 24424-99-5
RGT CA 121-44-8 Et3N
PRO CP 323191-90-8
CAT 1122-58-3 4-DMAP
SOL 109-99-9 THF

RX(36) RCT CP 323191-90-8

STAGE(1)

RGT CA 121-44-8 Et3N, CJ 541-41-3 ClCO2Et
SOL 109-99-9 THF

STAGE(2)

RGT CK 16940-66-2 NaBH4

STAGE(3)

RGT O 7647-01-0 HCl
SOL 7732-18-5 Water

PRO CQ 396725-71-6

RX(37) RCT CQ 396725-71-6

STAGE(1)

RGT CM 79-37-8 (COCl)2, CN 67-68-5 DMSO
SOL 75-09-2 CH2Cl2

STAGE(2)

RGT CA 121-44-8 Et3N

PRO CR 396725-72-7

RX(38) RCT CR 396725-72-7, AT 191103-10-3

STAGE(1)

CAT 64-19-7 AcOH

SOL 75-09-2 CH2Cl2

STAGE(2)

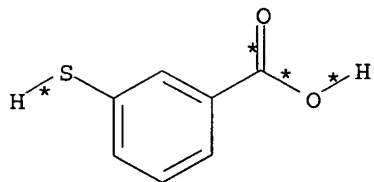
RGT CK 16940-66-2 NaBH4

PRO BM 396725-73-8

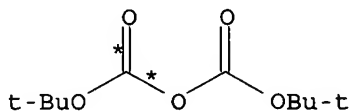
NTE in-situ generated reactant

RX(203) OF 350 COMPOSED OF RX(35), RX(36), RX(37), RX(39)

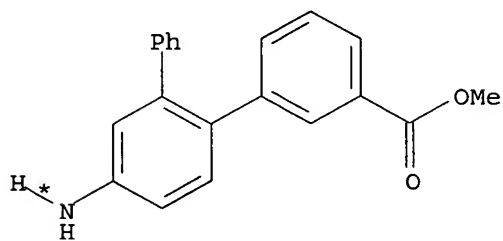
RX(203) CO + CF + AQ ==> BO



CO

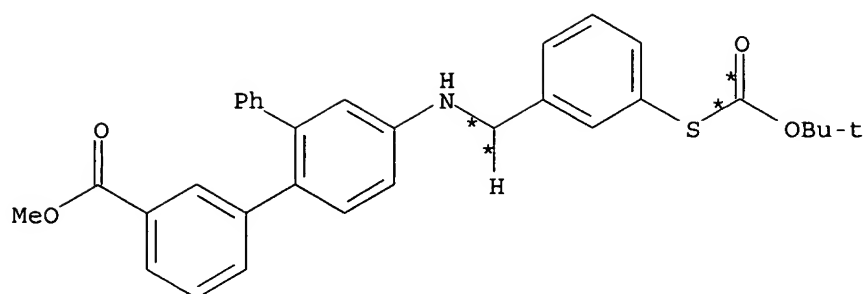


CF



AQ

4
STEPS
→



BO
YIELD 50%

RX(35) RCT CO 4869-59-4, CF **24424-99-5**
RGT CA 121-44-8 Et3N
PRO CP 323191-90-8
CAT 1122-58-3 4-DMAP
SOL 109-99-9 THF

RX(36) RCT CP 323191-90-8

STAGE(1)

RGT CA 121-44-8 Et3N, CJ 541-41-3 ClCO2Et
SOL 109-99-9 THF

STAGE(2)

RGT CK 16940-66-2 NaBH4

STAGE(3)

RGT O 7647-01-0 HCl
SOL 7732-18-5 Water

PRO CQ 396725-71-6

RX(37) RCT CQ 396725-71-6

STAGE(1)

RGT CM 79-37-8 (COCl)2, CN 67-68-5 DMSO
SOL 75-09-2 CH2Cl2

STAGE(2)

RGT CA 121-44-8 Et3N

PRO CR 396725-72-7

RX(39) RCT CR 396725-72-7, AQ **396725-50-1**

STAGE(1)

CAT 64-19-7 AcOH
SOL 75-09-2 CH2Cl2

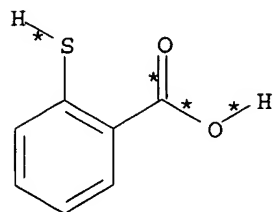
STAGE(2)

RGT CK 16940-66-2 NaBH4

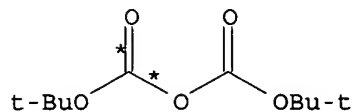
PRO BO **396725-74-9**

NTE in-situ generated reactant

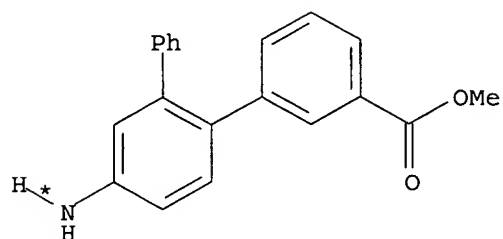
RX(212) OF 350 COMPOSED OF RX(40), RX(41), RX(42), RX(43)
 RX(212) CS + CF + AQ ==> BU



CS

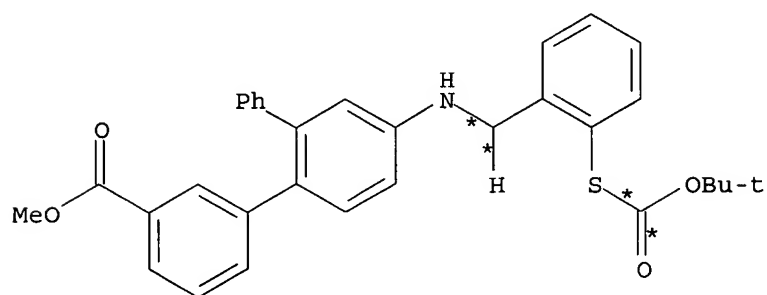


CF



AQ

4
 STEPS
 →



BU

YIELD 64%

RX(40) RCT CS 147-93-3, CF 24424-99-5
 RGT CA 121-44-8 Et3N
 PRO CT 396725-75-0
 CAT 1122-58-3 4-DMAP
 SOL 109-99-9 THF

RX(41) RCT CT 396725-75-0

STAGE(1)

RGT CA 121-44-8 Et3N, CJ 541-41-3 ClCO2Et
 SOL 109-99-9 THF

STAGE(2)

RGT CK 16940-66-2 NaBH4

STAGE(3)

RGT O 7647-01-0 HCl

SOL 7732-18-5 Water

PRO CU 396725-76-1

RX(42) RCT CU 396725-76-1

STAGE(1)

RGT CM 79-37-8 (COCl)2, CN 67-68-5 DMSO

SOL 75-09-2 CH2Cl2

STAGE(2)

RGT CA 121-44-8 Et3N

PRO CV 396725-77-2

RX(43) RCT CV 396725-77-2, AQ 396725-50-1

STAGE(1)

CAT 64-19-7 AcOH

SOL 75-09-2 CH2Cl2

STAGE(2)

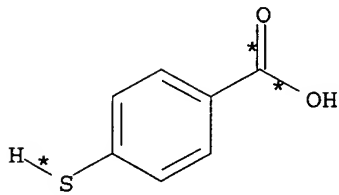
RGT CK 16940-66-2 NaBH4

PRO BU 396725-78-3

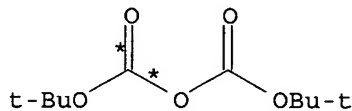
NTE in-situ generated reactant

RX(330) OF 350 COMPOSED OF RX(30), RX(31), RX(32), RX(33), RX(21)

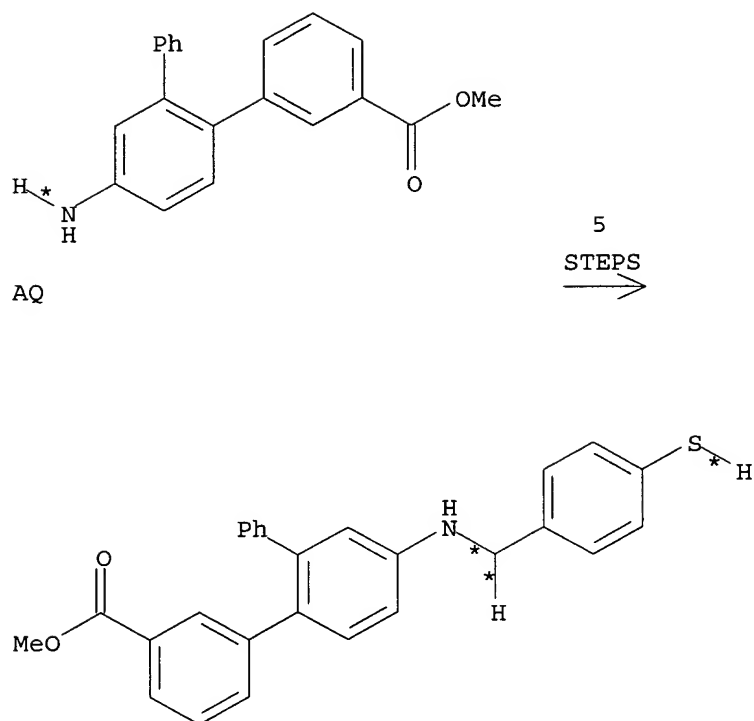
RX(330) CE + CF + AQ ==> BL



CE



CF



BL
YIELD 100%

RX(30) RCT CE 1074-36-8, CF 24424-99-5
RGT CA 121-44-8 Et₃N
PRO CG 396725-66-9
CAT 1122-58-3 4-DMAP
SOL 109-99-9 THF

RX(31) RCT CG 396725-66-9

STAGE(1)

RGT CA 121-44-8 Et₃N, CJ 541-41-3 ClCO₂Et
SOL 109-99-9 THF

STAGE(2)

RGT CK 16940-66-2 NaBH₄

STAGE(3)

RGT O 7647-01-0 HCl
SOL 7732-18-5 Water

PRO CI 396725-67-0

RX(32) RCT CI 396725-67-0

STAGE(1)

RGT CM 79-37-8 (COCl)₂, CN 67-68-5 DMSO
SOL 75-09-2 CH₂Cl₂

STAGE(2)

RGT CA 121-44-8 Et3N

PRO CL 396725-68-1

RX(33) RCT CL 396725-68-1, AQ 396725-50-1

STAGE(1)

CAT 64-19-7 AcOH

SOL 75-09-2 CH2Cl2

STAGE(2)

RGT CK 16940-66-2 NaBH4

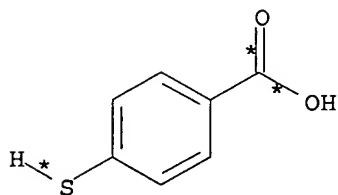
PRO BK 396725-69-2

NTE in-situ generated reactant

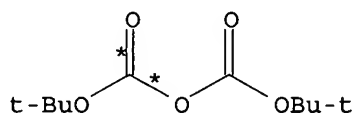
RX(21) RCT BK 396725-69-2
RGT B 76-05-1 F3CCO2H
PRO BL 396725-60-3
SOL 75-09-2 CH2Cl2

RX(331) OF 350 COMPOSED OF RX(30), RX(31), RX(32), RX(34), RX(20)

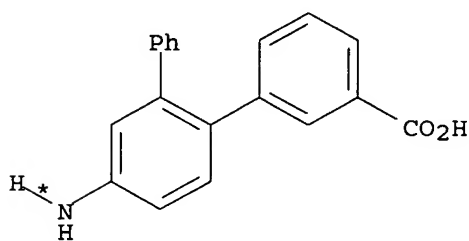
RX(331) CE + CF + AT ==> BI



CE

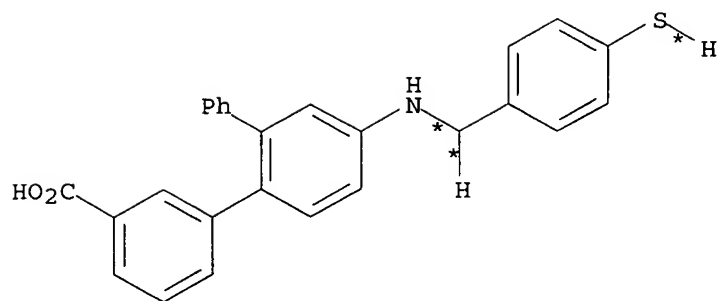


CF



AT

5
STEPS
→



BI
YIELD 87%

RX(30) RCT CE 1074-36-8, CF **24424-99-5**
 RGT CA 121-44-8 Et3N
 PRO CG 396725-66-9
 CAT 1122-58-3 4-DMAP
 SOL 109-99-9 THF

RX(31) RCT CG 396725-66-9

STAGE(1)
 RGT CA 121-44-8 Et3N, CJ 541-41-3 ClCO2Et
 SOL 109-99-9 THF

STAGE(2)
 RGT CK 16940-66-2 NaBH4

STAGE(3)
 RGT O 7647-01-0 HCl
 SOL 7732-18-5 Water

PRO CI 396725-67-0

RX(32) RCT CI 396725-67-0

STAGE(1)
 RGT CM 79-37-8 (COCl)2, CN 67-68-5 DMSO
 SOL 75-09-2 CH2Cl2

STAGE(2)
 RGT CA 121-44-8 Et3N

PRO CL 396725-68-1

RX(34) RCT CL 396725-68-1, AT **191103-10-3**

STAGE(1)
 CAT 64-19-7 AcOH
 SOL 75-09-2 CH2Cl2

STAGE(2)
 RGT CK 16940-66-2 NaBH4

PRO BH 396725-70-5

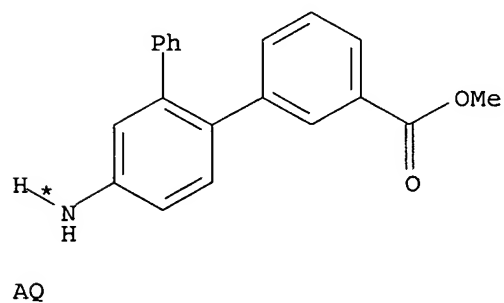
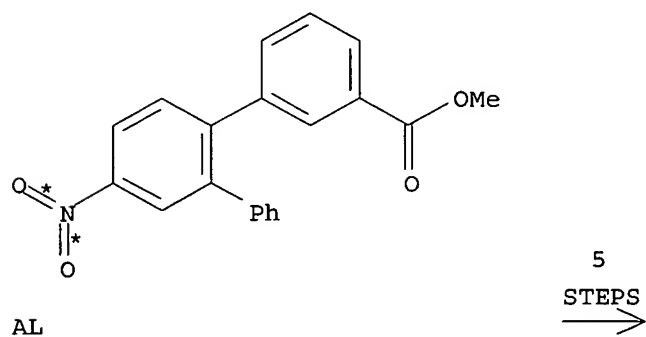
NTE in-situ generated reactant

RX(20) RCT BH 396725-70-5
 RGT B 76-05-1 F3CCO2H
 PRO BI 396725-59-0
 SOL 75-09-2 CH2Cl2

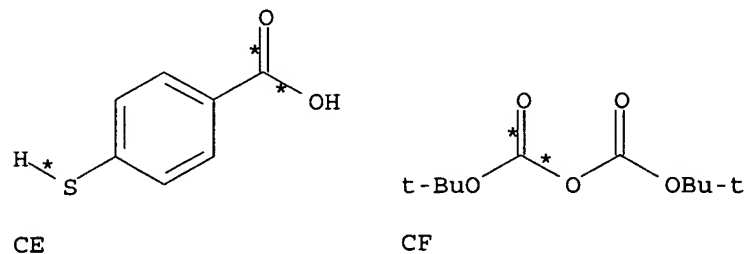
RX(332) OF 350 COMPOSED OF REACTION SEQUENCE RX(10), RX(33), RX(21)
 AND REACTION SEQUENCE RX(30), RX(31), RX(32), RX(33), RX(21)

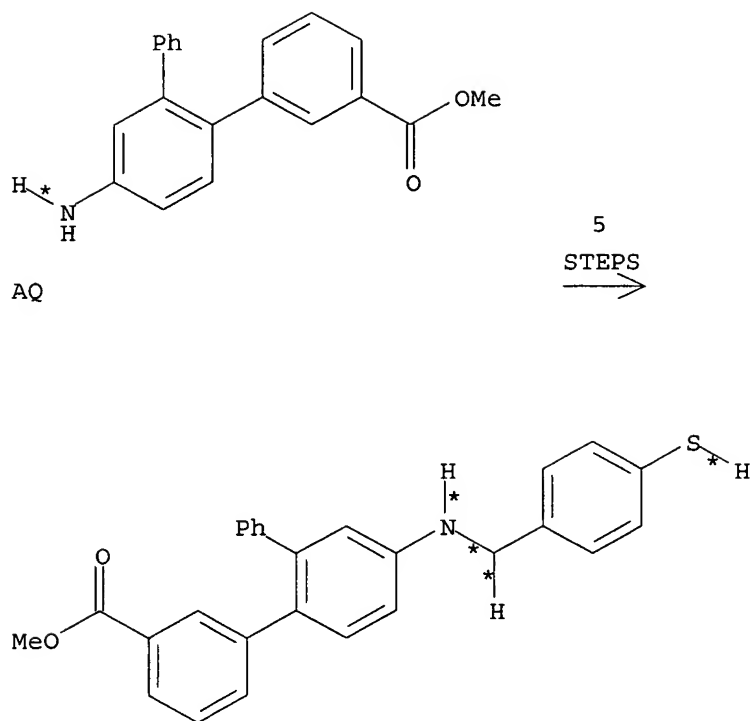
...AL ==> AQ...

...CE + CF + AQ ==> BL



START NEXT REACTION SEQUENCE





AQ

5
STEPS
→BL
YIELD 100%

RX(10) RCT AL 323191-84-0
 RGT AR 7772-99-8 SnCl₂
 PRO AQ 396725-50-1
 SOL 141-78-6 AcOEt

RX(30) RCT CE 1074-36-8, CF 24424-99-5
 RGT CA 121-44-8 Et₃N
 PRO CG 396725-66-9
 CAT 1122-58-3 4-DMAP
 SOL 109-99-9 THF

RX(31) RCT CG 396725-66-9

STAGE(1)
 RGT CA 121-44-8 Et₃N, CJ 541-41-3 ClCO₂Et
 SOL 109-99-9 THF

STAGE(2)
 RGT CK 16940-66-2 NaBH₄

STAGE(3)
 RGT O 7647-01-0 HCl
 SOL 7732-18-5 Water

PRO CI 396725-67-0

RX(32) RCT CI 396725-67-0

STAGE(1)

RGT CM 79-37-8 (COCl)₂, CN 67-68-5 DMSO
 SOL 75-09-2 CH₂Cl₂

STAGE(2)

RGT CA 121-44-8 Et₃N

PRO CL 396725-68-1

RX(33) RCT CL 396725-68-1, AQ 396725-50-1

STAGE(1)

CAT 64-19-7 AcOH
 SOL 75-09-2 CH₂Cl₂

STAGE(2)

RGT CK 16940-66-2 NaBH₄

PRO BK 396725-69-2

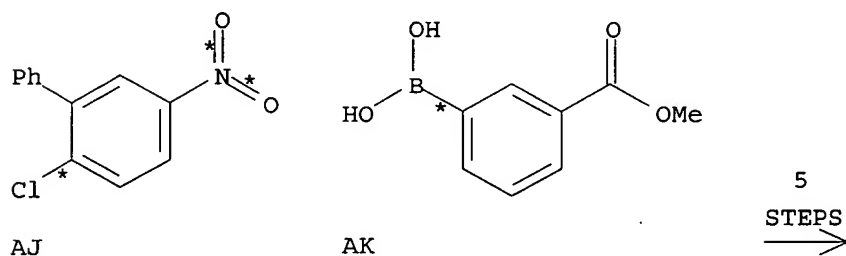
NTE in-situ generated reactant

RX(21) RCT BK 396725-69-2
 RGT B 76-05-1 F₃CCO₂H
 PRO BL 396725-60-3
 SOL 75-09-2 CH₂Cl₂

RX(333) OF 350 COMPOSED OF REACTION SEQUENCE RX(9), RX(10), RX(33), RX(21)
 AND REACTION SEQUENCE RX(30), RX(31), RX(32), RX(33), RX(21)

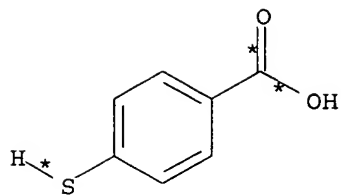
...AJ + AK ==> AQ...

...CE + CF + AQ ==> BL

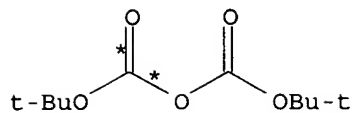


AQ

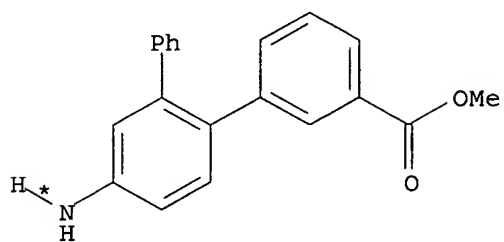
START NEXT REACTION SEQUENCE



CE

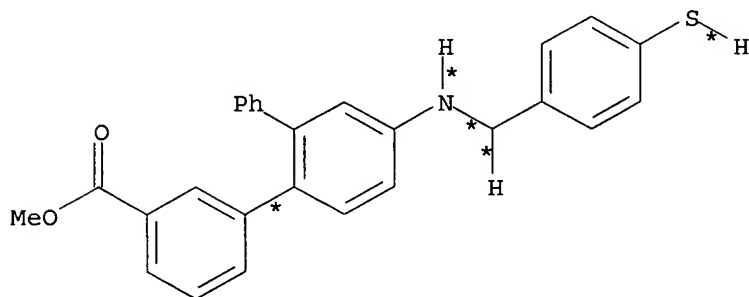


CF



AQ

5
STEPS
→



BL

YIELD 100%

RX(9) RCT AJ 29608-76-2, AK 99769-19-4
 RGT AM 7778-53-2 K3PO4, AN 247940-06-3 Phosphine,
 [1,1'-biphenyl]-2-ylidicyclohexyl-
 PRO AL 323191-84-0
 CAT 3375-31-3 Pd(OAc)2
 SOL 108-88-3 PhMe

RX(10) RCT AL 323191-84-0
 RGT AR 7772-99-8 SnCl2
 PRO AQ 396725-50-1
 SOL 141-78-6 AcOEt

RX(30) RCT CE 1074-36-8, CF 24424-99-5
 RGT CA 121-44-8 Et3N
 PRO CG 396725-66-9

CAT 1122-58-3 4-DMAP
SOL 109-99-9 THF

RX(31) RCT CG 396725-66-9

STAGE(1)
RGT CA 121-44-8 Et3N, CJ 541-41-3 ClCO2Et
SOL 109-99-9 THF

STAGE(2)
RGT CK 16940-66-2 NaBH4

STAGE(3)
RGT O 7647-01-0 HCl
SOL 7732-18-5 Water

PRO CI 396725-67-0

RX(32) RCT CI 396725-67-0

STAGE(1)
RGT CM 79-37-8 (COCl)2, CN 67-68-5 DMSO
SOL 75-09-2 CH2Cl2

STAGE(2)
RGT CA 121-44-8 Et3N

PRO CL 396725-68-1

RX(33) RCT CL 396725-68-1, AQ 396725-50-1

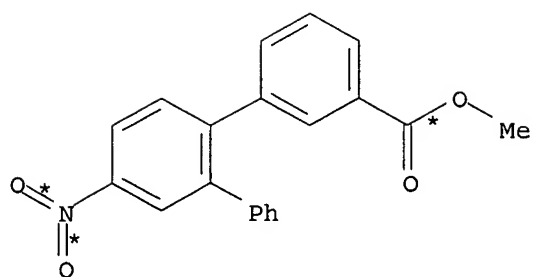
STAGE(1)
CAT 64-19-7 AcOH
SOL 75-09-2 CH2Cl2

STAGE(2)
RGT CK 16940-66-2 NaBH4

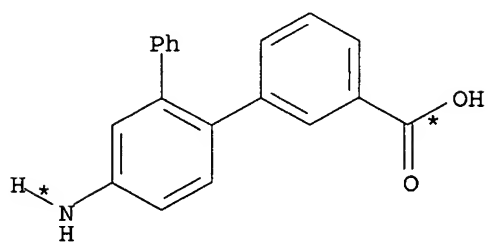
PRO BK 396725-69-2
NTE in-situ generated reactant

RX(21) RCT BK 396725-69-2
RGT B 76-05-1 F3CCO2H
PRO BL 396725-60-3
SOL 75-09-2 CH2Cl2

RX(334) OF 350 COMPOSED OF REACTION SEQUENCE RX(11), RX(34), RX(20)
AND REACTION SEQUENCE RX(30), RX(31), RX(32), RX(34), RX(20)
...AL ==> AT...
...CE + CF + AT ==> BI

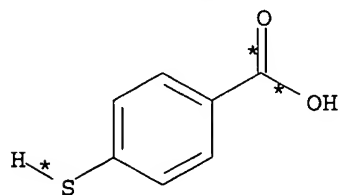


AL

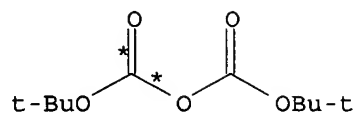
5
STEPS
→

AT

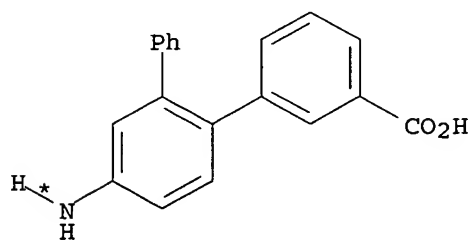
START NEXT REACTION SEQUENCE



CE

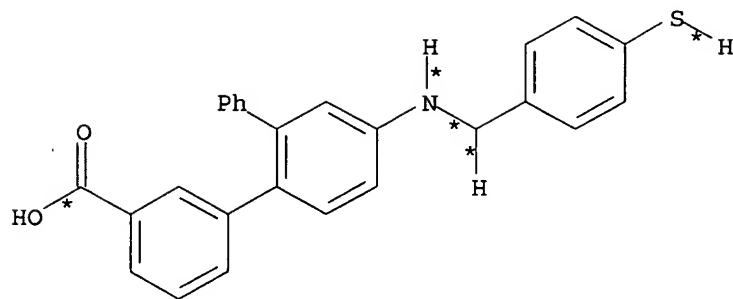


CF



AT

5
STEPS
→



BI
YIELD 87%

RX(11) RCT AL 323191-84-0

STAGE(1)

RGT AU 1310-65-2 LiOH

SOL 109-99-9 THF, 7732-18-5 Water

STAGE(2)

RGT AR 7772-99-8 SnCl₂

SOL 141-78-6 AcOEt

PRO AT 191103-10-3

RX(30) RCT CE 1074-36-8, CF 24424-99-5

RGT CA 121-44-8 Et₃N

PRO CG 396725-66-9

CAT 1122-58-3 4-DMAP

SOL 109-99-9 THF

RX(31) RCT CG 396725-66-9

STAGE(1)

RGT CA 121-44-8 Et₃N, CJ 541-41-3 ClCO₂Et

SOL 109-99-9 THF

STAGE(2)

RGT CK 16940-66-2 NaBH₄

STAGE(3)

RGT O 7647-01-0 HCl

SOL 7732-18-5 Water

PRO CI 396725-67-0

RX(32) RCT CI 396725-67-0

STAGE(1)

RGT CM 79-37-8 (COCl)₂, CN 67-68-5 DMSO

SOL 75-09-2 CH₂Cl₂

STAGE(2)

RGT CA 121-44-8 Et₃N

PRO CL 396725-68-1

RX(34) RCT CL 396725-68-1, AT 191103-10-3

STAGE(1)

CAT 64-19-7 AcOH

SOL 75-09-2 CH₂Cl₂

STAGE(2)

RGT CK 16940-66-2 NaBH₄

PRO BH 396725-70-5

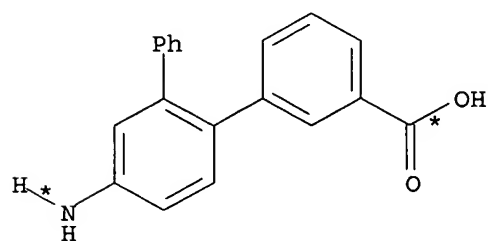
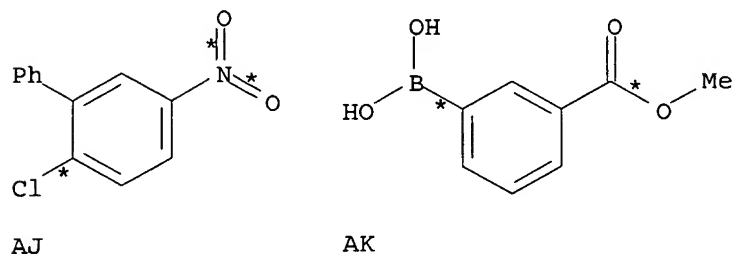
NTE in-situ generated reactant

RX(20) RCT BH 396725-70-5
 RGT B 76-05-1 F₃CCO₂H
 PRO BI 396725-59-0
 SOL 75-09-2 CH₂Cl₂

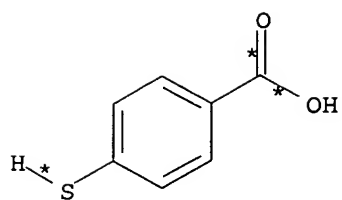
RX(335) OF 350 COMPOSED OF REACTION SEQUENCE RX(9), RX(11), RX(34), RX(20)
 AND REACTION SEQUENCE RX(30), RX(31), RX(32), RX(34), RX(20)

...AJ + AK ==> AT...

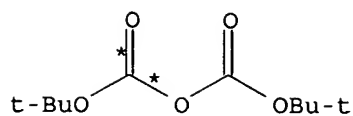
...CE + CF + AT ==> BI



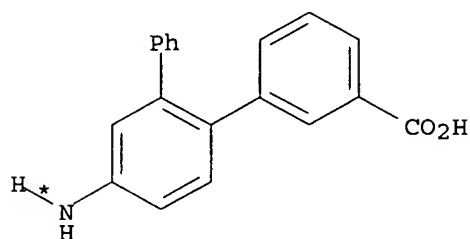
START NEXT REACTION SEQUENCE



CE

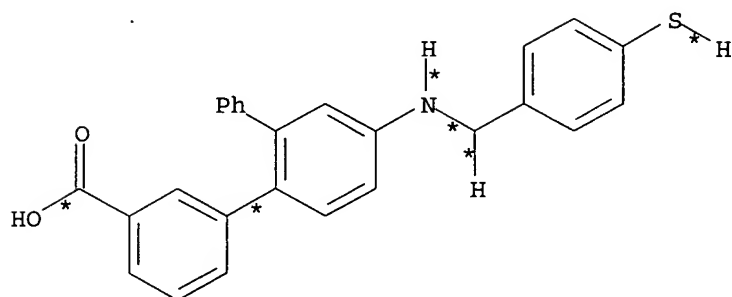


CF



AT

5
STEPS
→



BI

YIELD 87%

RX(9) RCT AJ 29608-76-2, AK 99769-19-4
 RGT AM 7778-53-2 K3PO4, AN 247940-06-3 Phosphine,
 [1,1'-biphenyl]-2-ylidicyclohexyl-
 PRO AL 323191-84-0
 CAT 3375-31-3 Pd(OAc)₂
 SOL 108-88-3 PhMe

RX(11) RCT AL 323191-84-0

STAGE(1)

RGT AU 1310-65-2 LiOH

SOL 109-99-9 THF, 7732-18-5 Water

STAGE(2)

RGT AR 7772-99-8 SnCl₂
SOL 141-78-6 AcOEt

PRO AT 191103-10-3

RX(30) RCT CE 1074-36-8, CF **24424-99-5**
RGT CA 121-44-8 Et₃N
PRO CG 396725-66-9
CAT 1122-58-3 4-DMAP
SOL 109-99-9 THF

RX(31) RCT CG 396725-66-9

STAGE(1)

RGT CA 121-44-8 Et₃N, CJ 541-41-3 ClCO₂Et
SOL 109-99-9 THF

STAGE(2)

RGT CK 16940-66-2 NaBH₄

STAGE(3)

RGT O 7647-01-0 HCl
SOL 7732-18-5 Water

PRO CI 396725-67-0

RX(32) RCT CI 396725-67-0

STAGE(1)

RGT CM 79-37-8 (COCl)₂, CN 67-68-5 DMSO
SOL 75-09-2 CH₂Cl₂

STAGE(2)

RGT CA 121-44-8 Et₃N

PRO CL 396725-68-1

RX(34) RCT CL 396725-68-1, AT **191103-10-3**

STAGE(1)

CAT 64-19-7 AcOH
SOL 75-09-2 CH₂Cl₂

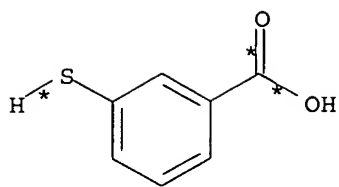
STAGE(2)

RGT CK 16940-66-2 NaBH₄

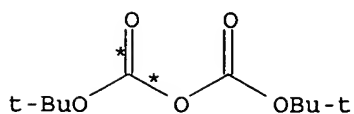
PRO BH 396725-70-5
NTE in-situ generated reactant

RX(20) RCT BH 396725-70-5
RGT B 76-05-1 F₃CCO₂H
PRO BI **396725-59-0**
SOL 75-09-2 CH₂Cl₂

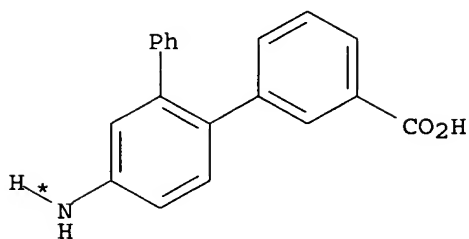
RX(336) OF 350 COMPOSED OF RX(35), RX(36), RX(37), RX(38), RX(22)
RX(336) CO + **CF** + **AT** ==> **BN**



CO

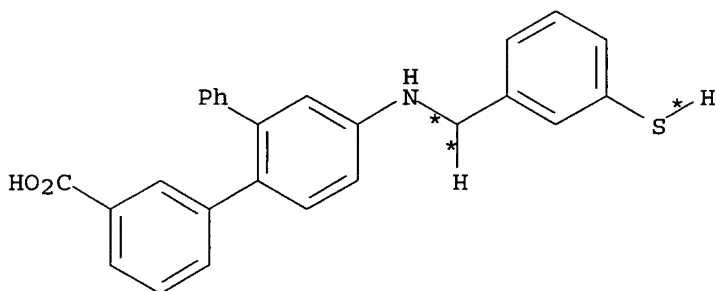


CF



AT

5
STEPS
→



BN

YIELD 88%

RX(35) RCT CO 4869-59-4, CF 24424-99-5
 RGT CA 121-44-8 Et3N
 PRO CP 323191-90-8
 CAT 1122-58-3 4-DMAP
 SOL 109-99-9 THF

RX(36) RCT CP 323191-90-8

STAGE(1)

RGT CA 121-44-8 Et3N, CJ 541-41-3 ClCO2Et
 SOL 109-99-9 THF

STAGE(2)

RGT CK 16940-66-2 NaBH4

STAGE(3)

RGT O 7647-01-0 HCl
SOL 7732-18-5 Water

PRO CQ 396725-71-6

RX(37) RCT CQ 396725-71-6

STAGE(1)

RGT CM 79-37-8 (COCl)₂, CN 67-68-5 DMSO
SOL 75-09-2 CH₂Cl₂

STAGE(2)

RGT CA 121-44-8 Et₃N

PRO CR 396725-72-7

RX(38) RCT CR 396725-72-7, AT 191103-10-3

STAGE(1)

CAT 64-19-7 AcOH
SOL 75-09-2 CH₂Cl₂

STAGE(2)

RGT CK 16940-66-2 NaBH₄

PRO BM 396725-73-8

NTE in-situ generated reactant

RX(22) RCT BM 396725-73-8

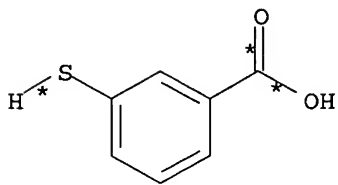
RGT B 76-05-1 F₃CCO₂H

PRO BN 396725-61-4

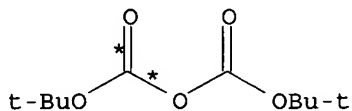
SOL 75-09-2 CH₂Cl₂

RX(337) OF 350 COMPOSED OF RX(35), RX(36), RX(37), RX(39), RX(23)

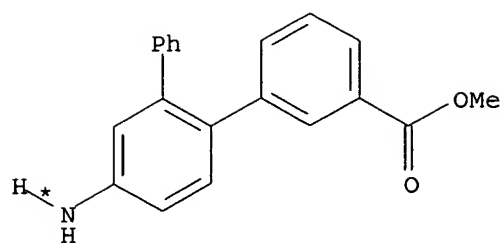
RX(337) CO + CF + AQ ==> BP



CO

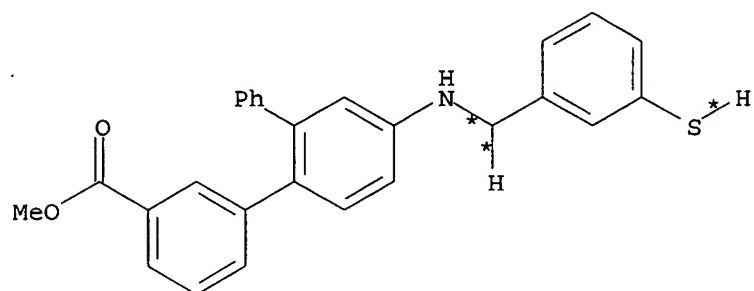


CF



AQ

5
STEPS
→



BP

YIELD 100%

RX(35) RCT CO 4869-59-4, CF 24424-99-5
RGT CA 121-44-8 Et₃N
PRO CP 323191-90-8
CAT 1122-58-3 4-DMAP
SOL 109-99-9 THF

RX(36) RCT CP 323191-90-8

STAGE(1)

RGT CA 121-44-8 Et₃N, CJ 541-41-3 ClCO₂Et
SOL 109-99-9 THF

STAGE(2)

RGT CK 16940-66-2 NaBH₄

STAGE(3)

RGT O 7647-01-0 HCl
SOL 7732-18-5 Water

PRO CQ 396725-71-6

RX(37) RCT CQ 396725-71-6

STAGE(1)

RGT CM 79-37-8 (COCl)₂, CN 67-68-5 DMSO
SOL 75-09-2 CH₂Cl₂

STAGE(2)

RGT CA 121-44-8 Et3N

PRO CR 396725-72-7

RX(39) RCT CR 396725-72-7, AQ 396725-50-1

STAGE(1)

CAT 64-19-7 AcOH

SOL 75-09-2 CH2Cl2

STAGE(2)

RGT CK 16940-66-2 NaBH4

PRO BO 396725-74-9

NTE in-situ generated reactant

RX(23) RCT BO 396725-74-9

RGT B 76-05-1 F3CCO2H

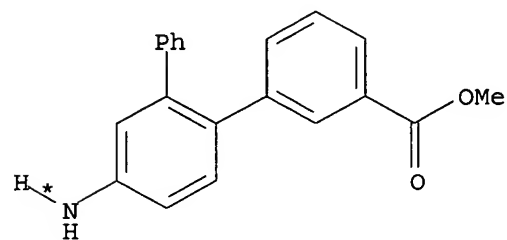
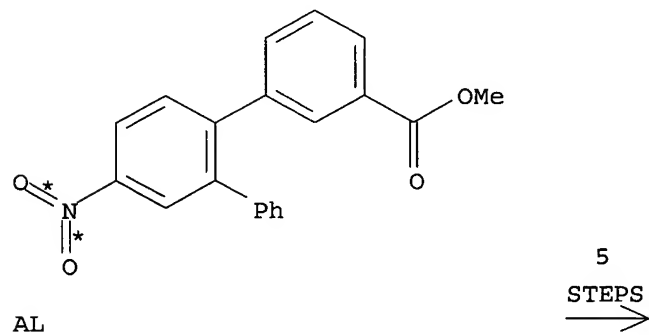
PRO BP 396725-62-5

SOL 75-09-2 CH2Cl2

RX(338) OF 350 COMPOSED OF REACTION SEQUENCE RX(10), RX(39), RX(23)
AND REACTION SEQUENCE RX(35), RX(36), RX(37), RX(39), RX(23)

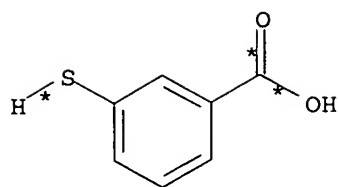
...AL ==> AQ...

...CO + CF + AQ ==> BP

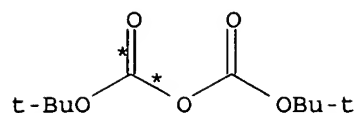


AQ

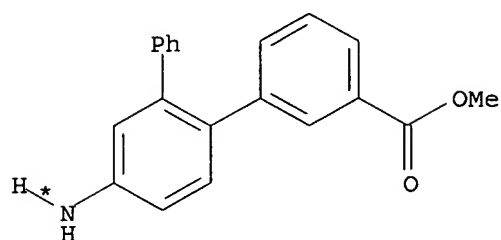
START NEXT REACTION SEQUENCE



CO

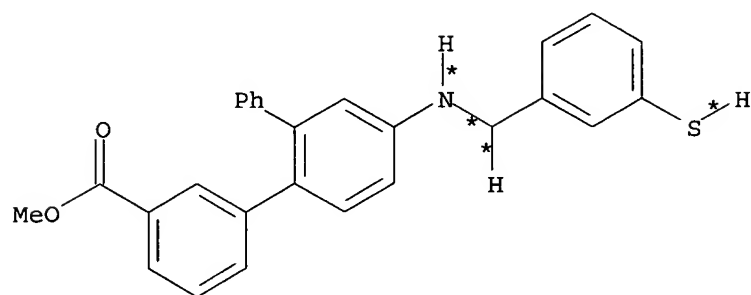


CF



AQ

5
STEPS
→



BP
YIELD 100%

RX(10) RCT AL 323191-84-0
RGT AR 7772-99-8 SnCl₂
PRO AQ 396725-50-1
SOL 141-78-6 AcOEt

RX(35) RCT CO 4869-59-4, CF 24424-99-5
RGT CA 121-44-8 Et₃N
PRO CP 323191-90-8
CAT 1122-58-3 4-DMAP
SOL 109-99-9 THF

RX(36) RCT CP 323191-90-8

STAGE(1)

RGT CA 121-44-8 Et₃N, CJ 541-41-3 ClCO₂Et

SOL 109-99-9 THF

STAGE(2)

RGT CK 16940-66-2 NaBH4

STAGE(3)

RGT O 7647-01-0 HCl

SOL 7732-18-5 Water

PRO CQ 396725-71-6

RX(37) RCT CQ 396725-71-6

STAGE(1)

RGT CM 79-37-8 (COCl)₂, CN 67-68-5 DMSO

SOL 75-09-2 CH₂Cl₂

STAGE(2)

RGT CA 121-44-8 Et₃N

PRO CR 396725-72-7

RX(39) RCT CR 396725-72-7, AQ 396725-50-1

STAGE(1)

CAT 64-19-7 AcOH

SOL 75-09-2 CH₂Cl₂

STAGE(2)

RGT CK 16940-66-2 NaBH₄

PRO BO 396725-74-9

NTE in-situ generated reactant

RX(23) RCT BO 396725-74-9

RGT B 76-05-1 F₃CCO₂H

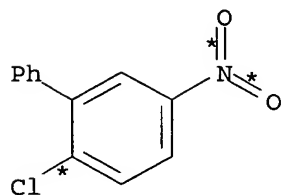
PRO BP 396725-62-5

SOL 75-09-2 CH₂Cl₂

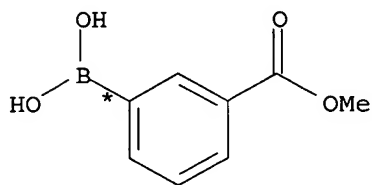
RX(339) OF 350 COMPOSED OF REACTION SEQUENCE RX(9), RX(10), RX(39), RX(23)
AND REACTION SEQUENCE RX(35), RX(36), RX(37), RX(39), RX(23)

...AJ + AK ==> AQ...

...CO + CF + AQ ==> BP

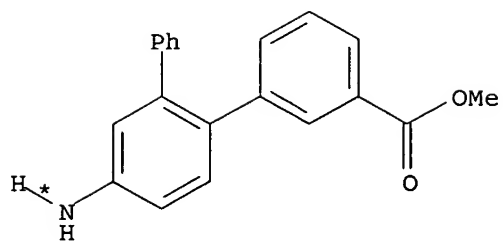


AJ



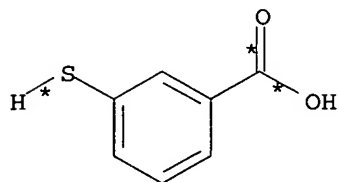
AK

5
STEPS
→

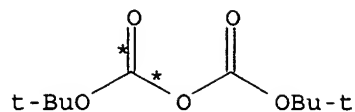


AQ

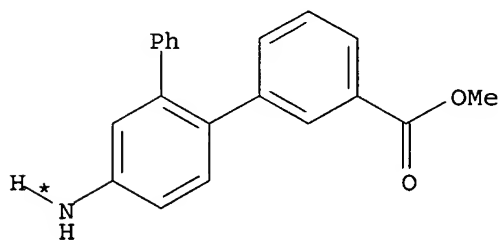
START NEXT REACTION SEQUENCE



CO

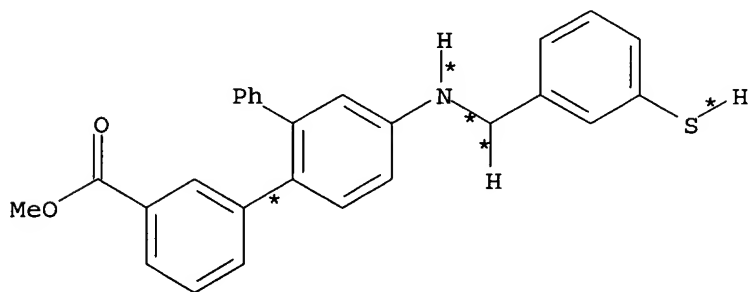


CF



AQ

5
STEPS
→



BP
YIELD 100%

RX(9) RCT AJ 29608-76-2, AK 99769-19-4

RGT AM 7778-53-2 K3PO4, AN 247940-06-3 Phosphine,
[1,1'-biphenyl]-2-ylidicyclohexyl-
PRO AL 323191-84-0
CAT 3375-31-3 Pd(OAc)2
SOL 108-88-3 PhMe

RX(10) RCT AL 323191-84-0
RGT AR 7772-99-8 SnCl2
PRO AQ 396725-50-1
SOL 141-78-6 AcOEt

RX(35) RCT CO 4869-59-4, CF **24424-99-5**
RGT CA 121-44-8 Et3N
PRO CP 323191-90-8
CAT 1122-58-3 4-DMAP
SOL 109-99-9 THF

RX(36) RCT CP 323191-90-8

STAGE(1)
RGT CA 121-44-8 Et3N, CJ 541-41-3 ClCO2Et
SOL 109-99-9 THF

STAGE(2)
RGT CK 16940-66-2 NaBH4

STAGE(3)
RGT O 7647-01-0 HCl
SOL 7732-18-5 Water

PRO CQ 396725-71-6

RX(37) RCT CQ 396725-71-6

STAGE(1)
RGT CM 79-37-8 (COCl)2, CN 67-68-5 DMSO
SOL 75-09-2 CH2Cl2

STAGE(2)
RGT CA 121-44-8 Et3N

PRO CR 396725-72-7

RX(39) RCT CR 396725-72-7, AQ **396725-50-1**

STAGE(1)
CAT 64-19-7 AcOH
SOL 75-09-2 CH2Cl2

STAGE(2)
RGT CK 16940-66-2 NaBH4

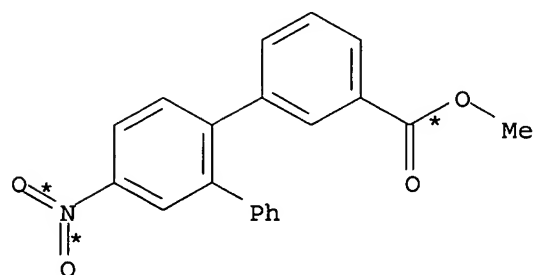
PRO BO 396725-74-9
NTE in-situ generated reactant

RX(23) RCT BO 396725-74-9
RGT B 76-05-1 F3CCO2H
PRO BP **396725-62-5**
SOL 75-09-2 CH2Cl2

RX(340) OF 350 COMPOSED OF REACTION SEQUENCE RX(11), RX(38), RX(22)
AND REACTION SEQUENCE RX(35), RX(36), RX(37), RX(38), RX(22)

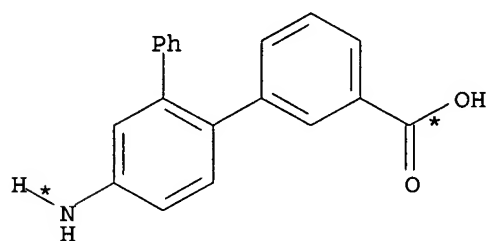
...AL ==> AT...

...CO + CF + AT ==> BN



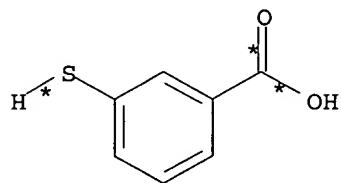
AL

5
STEPS
→

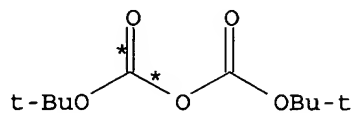


AT

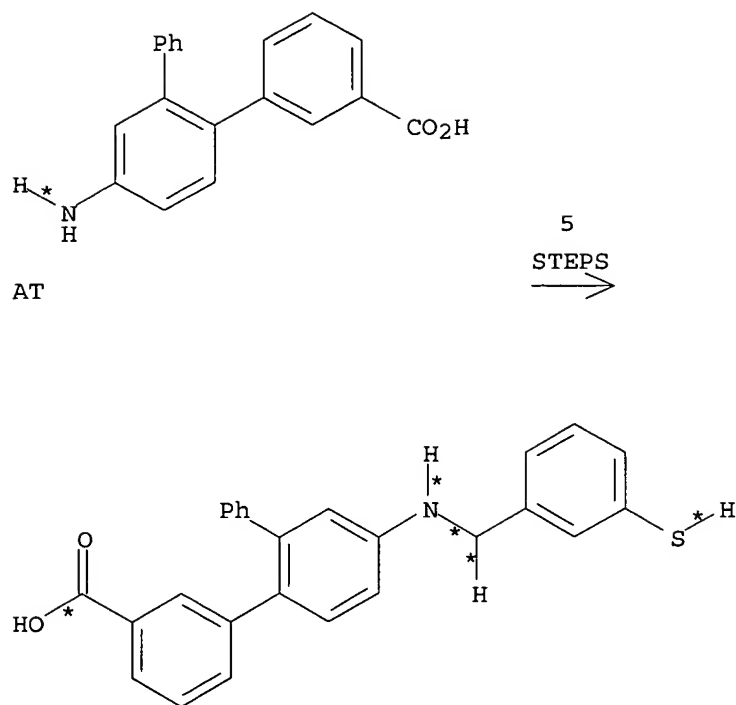
START NEXT REACTION SEQUENCE



CO



CF



BN
YIELD 88%

RX(11) RCT AL 323191-84-0

STAGE(1)

RGT AU 1310-65-2 LiOH
SOL 109-99-9 THF, 7732-18-5 Water

STAGE(2)

RGT AR 7772-99-8 SnCl₂
SOL 141-78-6 AcOEt

PRO AT 191103-10-3

RX(35) RCT CO 4869-59-4, CF **24424-99-5**
RGT CA 121-44-8 Et₃N
PRO CP 323191-90-8
CAT 1122-58-3 4-DMAP
SOL 109-99-9 THF

RX(36) RCT CP 323191-90-8

STAGE(1)

RGT CA 121-44-8 Et₃N, CJ 541-41-3 ClCO₂Et
SOL 109-99-9 THF

STAGE(2)

RGT CK 16940-66-2 NaBH₄

STAGE(3)

RGT O 7647-01-0 HCl
SOL 7732-18-5 Water

PRO CQ 396725-71-6

RX(37) RCT CQ 396725-71-6

STAGE(1)

RGT CM 79-37-8 (COCl)₂, CN 67-68-5 DMSO
SOL 75-09-2 CH₂Cl₂

STAGE(2)

RGT CA 121-44-8 Et₃N

PRO CR 396725-72-7

RX(38) RCT CR 396725-72-7, AT 191103-10-3

STAGE(1)

CAT 64-19-7 AcOH
SOL 75-09-2 CH₂Cl₂

STAGE(2)

RGT CK 16940-66-2 NaBH₄

PRO BM 396725-73-8

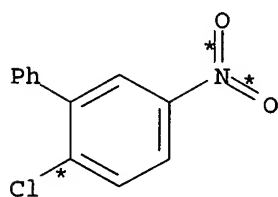
NTE in-situ generated reactant

RX(22) RCT BM 396725-73-8
RGT B 76-05-1 F₃CCO₂H
PRO BN 396725-61-4
SOL 75-09-2 CH₂Cl₂

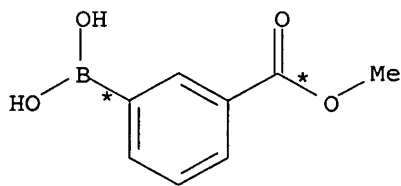
RX(341) OF 350 COMPOSED OF REACTION SEQUENCE RX(9), RX(11), RX(38), RX(22)
AND REACTION SEQUENCE RX(35), RX(36), RX(37), RX(38), RX(22)

...AJ + AK ==> AT...

...CO + CF + AT ==> BN

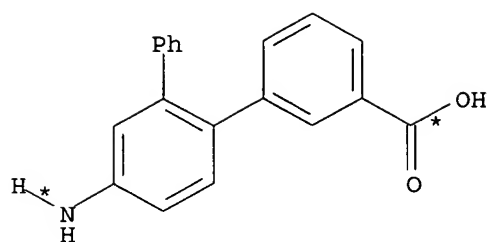


AJ



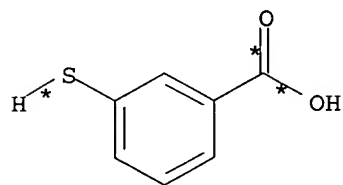
AK

5
STEPS
→

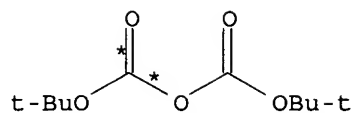


AT

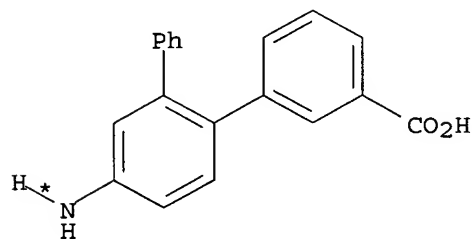
START NEXT REACTION SEQUENCE



CO

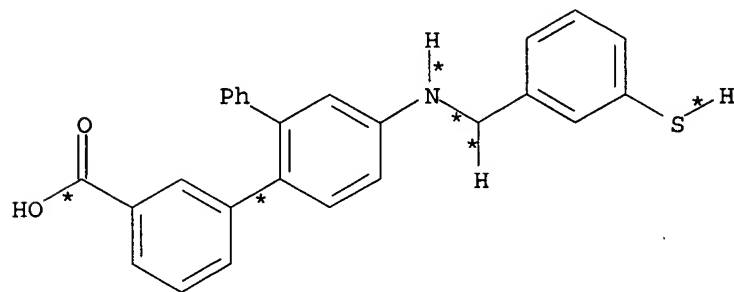


CF



AT

5
STEPS
→



BN
YIELD 88%

RX(9) RCT AJ 29608-76-2, AK 99769-19-4

RGT AM 7778-53-2 K3PO4, AN 247940-06-3 Phosphine,
[1,1'-biphenyl]-2-ylidicyclohexyl-
PRO AL 323191-84-0
CAT 3375-31-3 Pd(OAc)2
SOL 108-88-3 PhMe

RX(11) RCT AL 323191-84-0

STAGE(1)
RGT AU 1310-65-2 LiOH
SOL 109-99-9 THF, 7732-18-5 Water

STAGE(2)
RGT AR 7772-99-8 SnCl2
SOL 141-78-6 AcOEt

PRO AT 191103-10-3

RX(35) RCT CO 4869-59-4, CF **24424-99-5**
RGT CA 121-44-8 Et3N
PRO CP 323191-90-8
CAT 1122-58-3 4-DMAP
SOL 109-99-9 THF

RX(36) RCT CP 323191-90-8

STAGE(1)
RGT CA 121-44-8 Et3N, CJ 541-41-3 ClCO2Et
SOL 109-99-9 THF

STAGE(2)
RGT CK 16940-66-2 NaBH4

STAGE(3)
RGT O 7647-01-0 HCl
SOL 7732-18-5 Water

PRO CQ 396725-71-6

RX(37) RCT CQ 396725-71-6

STAGE(1)
RGT CM 79-37-8 (COCl)2, CN 67-68-5 DMSO
SOL 75-09-2 CH2Cl2

STAGE(2)
RGT CA 121-44-8 Et3N

PRO CR 396725-72-7

RX(38) RCT CR 396725-72-7, AT **191103-10-3**

STAGE(1)
CAT 64-19-7 AcOH
SOL 75-09-2 CH2Cl2

STAGE(2)
RGT CK 16940-66-2 NaBH4

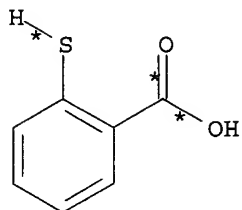
PRO BM 396725-73-8

NTE in-situ generated reactant

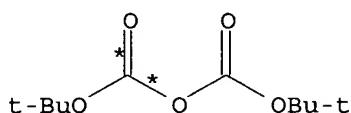
RX(22) RCT BM 396725-73-8
 RGT B 76-05-1 F3CCO2H
 PRO BN 396725-61-4
 SOL 75-09-2 CH2Cl2

RX(342) OF 350 COMPOSED OF RX(40), RX(41), RX(42), RX(43), RX(26)

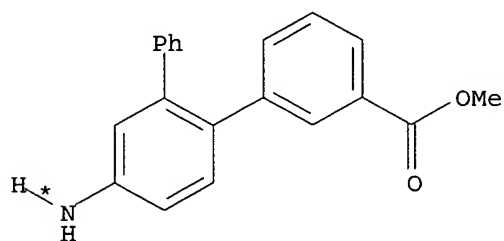
RX(342) CS + CF + AQ ==> BV



CS

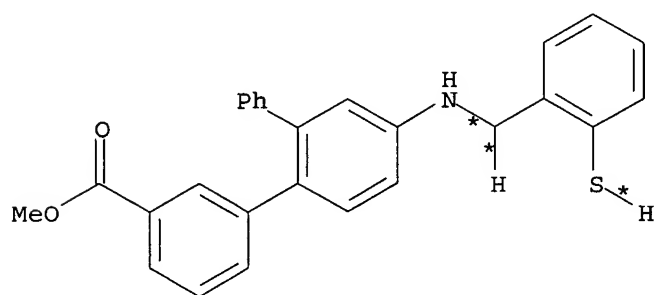


CF



AQ

5
 STEPS
 →



BV
 YIELD 100%

RX(40) RCT CS 147-93-3, CF 24424-99-5
 RGT CA 121-44-8 Et3N
 PRO CT 396725-75-0

CAT 1122-58-3 4-DMAP
SOL 109-99-9 THF

RX(41) RCT CT 396725-75-0

STAGE(1)

RGT CA 121-44-8 Et3N, CJ 541-41-3 ClCO2Et
SOL 109-99-9 THF

STAGE(2)

RGT CK 16940-66-2 NaBH4

STAGE(3)

RGT O 7647-01-0 HCl
SOL 7732-18-5 Water

PRO CU 396725-76-1

RX(42) RCT CU 396725-76-1

STAGE(1)

RGT CM 79-37-8 (COCl)2, CN 67-68-5 DMSO
SOL 75-09-2 CH2Cl2

STAGE(2)

RGT CA 121-44-8 Et3N

PRO CV 396725-77-2

RX(43) RCT CV 396725-77-2, AQ 396725-50-1

STAGE(1)

CAT 64-19-7 AcOH
SOL 75-09-2 CH2Cl2

STAGE(2)

RGT CK 16940-66-2 NaBH4

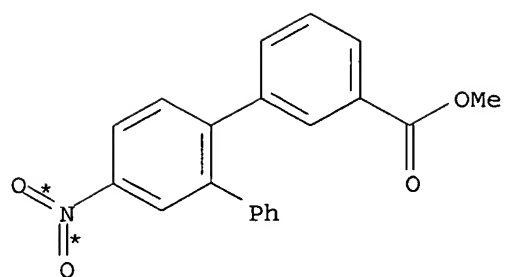
PRO BU 396725-78-3
NTE in-situ generated reactant

RX(26) RCT BU 396725-78-3
RGT B 76-05-1 F3CCO2H
PRO BV 396725-64-7
SOL 75-09-2 CH2Cl2

RX(343) OF 350 COMPOSED OF REACTION SEQUENCE RX(10), RX(43), RX(26)
AND REACTION SEQUENCE RX(40), RX(41), RX(42), RX(43), RX(26)

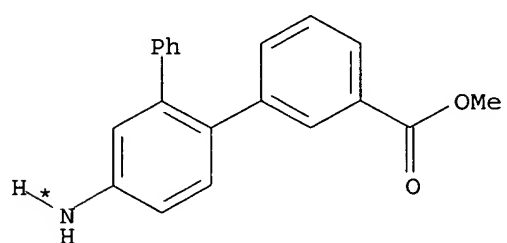
...AL ==> AQ...

...CS + CF + AQ ==> BV



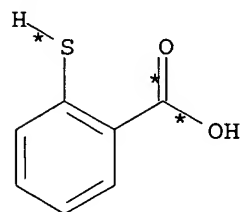
AL

5
STEPS
→

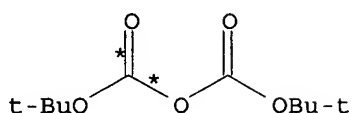


AQ

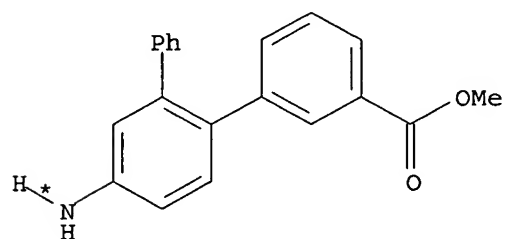
START NEXT REACTION SEQUENCE



CS

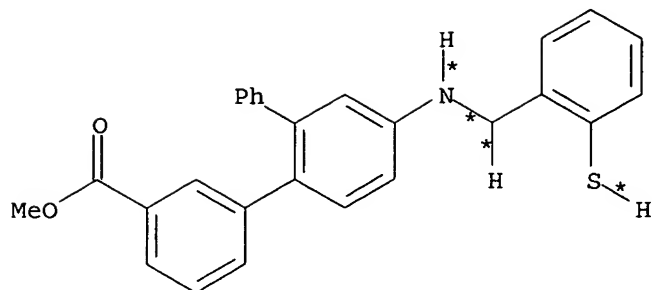


CF



AQ

5
STEPS
→



BV
YIELD 100%

RX(10) RCT AL 323191-84-0
RGT AR 7772-99-8 SnCl₂
PRO AQ 396725-50-1
SOL 141-78-6 AcOEt

RX(40) RCT CS 147-93-3, CF **24424-99-5**
RGT CA 121-44-8 Et₃N
PRO CT 396725-75-0
CAT 1122-58-3 4-DMAP
SOL 109-99-9 THF

RX(41) RCT CT 396725-75-0

STAGE(1)
RGT CA 121-44-8 Et₃N, CJ 541-41-3 ClCO₂Et
SOL 109-99-9 THF

STAGE(2)
RGT CK 16940-66-2 NaBH₄

STAGE(3)
RGT O 7647-01-0 HCl
SOL 7732-18-5 Water

PRO CU 396725-76-1

RX(42) RCT CU 396725-76-1

STAGE(1)
RGT CM 79-37-8 (COCl)₂, CN 67-68-5 DMSO
SOL 75-09-2 CH₂Cl₂

STAGE(2)
RGT CA 121-44-8 Et₃N

PRO CV 396725-77-2

RX(43) RCT CV 396725-77-2, AQ **396725-50-1**

STAGE(1)
CAT 64-19-7 AcOH
SOL 75-09-2 CH₂Cl₂

STAGE(2)

RGT CK 16940-66-2 NaBH4

PRO BU 396725-78-3

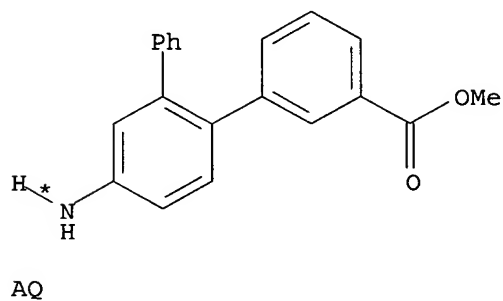
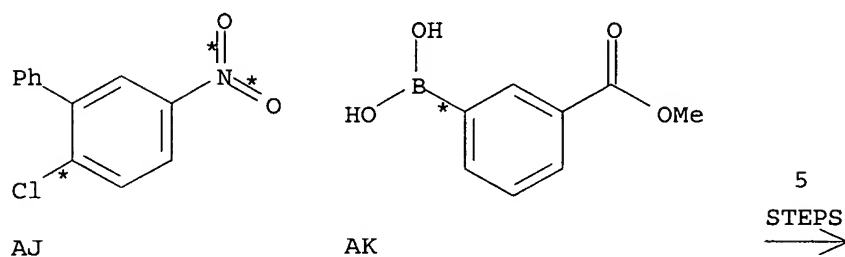
NTE in-situ generated reactant

RX(26) RCT BU 396725-78-3
 RGT B 76-05-1 F3CCO2H
 PRO BV 396725-64-7
 SOL 75-09-2 CH2Cl2

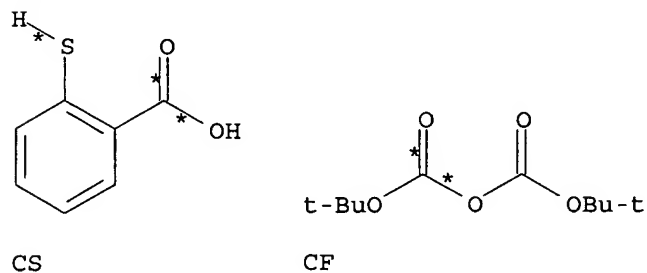
RX(344) OF 350 COMPOSED OF REACTION SEQUENCE RX(9), RX(10), RX(43), RX(26)
 AND REACTION SEQUENCE RX(40), RX(41), RX(42), RX(43), RX(26)

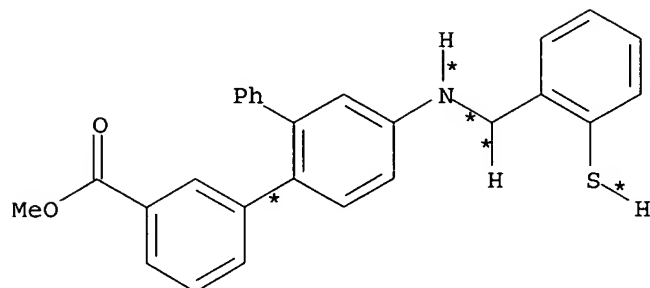
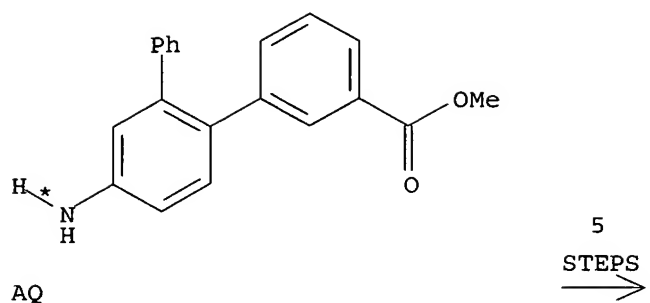
...AJ + AK ==> AQ...

...CS + CF + AQ ==> BV



START NEXT REACTION SEQUENCE





RX(9) RCT AJ 29608-76-2, AK 99769-19-4
 RGT AM 7778-53-2 K3PO4, AN 247940-06-3 Phosphine,
 [1,1'-biphenyl]-2-ylidicyclohexyl-
 PRO AL 323191-84-0
 CAT 3375-31-3 Pd(OAc)2
 SOL 108-88-3 PhMe

RX(10) RCT AL 323191-84-0
 RGT AR 7772-99-8 SnCl2
 PRO AQ 396725-50-1
 SOL 141-78-6 AcOEt

RX(40) RCT CS 147-93-3, CF 24424-99-5
 RGT CA 121-44-8 Et3N
 PRO CT 396725-75-0
 CAT 1122-58-3 4-DMAP
 SOL 109-99-9 THF

RX(41) RCT CT 396725-75-0

STAGE(1)

RGT CA 121-44-8 Et3N, CJ 541-41-3 ClCO2Et
 SOL 109-99-9 THF

STAGE(2)

RGT CK 16940-66-2 NaBH4

STAGE(3)

RGT O 7647-01-0 HCl
SOL 7732-18-5 Water

PRO CU 396725-76-1

RX(42) RCT CU 396725-76-1

STAGE(1)
RGT CM 79-37-8 (COCl)₂, CN 67-68-5 DMSO
SOL 75-09-2 CH₂Cl₂

STAGE(2)
RGT CA 121-44-8 Et₃N

PRO CV 396725-77-2

RX(43) RCT CV 396725-77-2, AQ 396725-50-1

STAGE(1)
CAT 64-19-7 AcOH
SOL 75-09-2 CH₂Cl₂

STAGE(2)
RGT CK 16940-66-2 NaBH₄

PRO BU 396725-78-3
NTE in-situ generated reactant

RX(26) RCT BU 396725-78-3
RGT B 76-05-1 F₃CCO₂H
PRO BV 396725-64-7
SOL 75-09-2 CH₂Cl₂

L60 ANSWER 26 OF 44 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 137:352757 CASREACT

TITLE: Catalytic Activity of Mesoporous Silica for Synthesis
of Methyl N-Phenyl Carbamate from Dimethyl Carbonate
and Aniline

AUTHOR(S): Katada, Naonobu; Fujinaga, Haruhisa; Nakamura,
Yukinori; Okumura, Kazu; Nishigaki, Kyoichi; Niwa,
Miki

CORPORATE SOURCE: Faculty of Engineering, Department of Materials
Science, Tottori University, Tottori, 680-8552, Japan

SOURCE: Catalysis Letters (2002), 80(1-2), 47-51

CODEN: CALEER; ISSN: 1011-372X

PUBLISHER: Kluwer Academic/Plenum Publishers

DOCUMENT TYPE: Journal

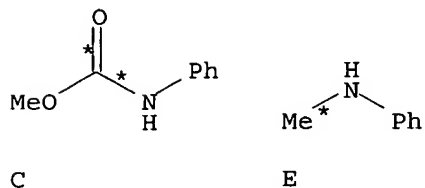
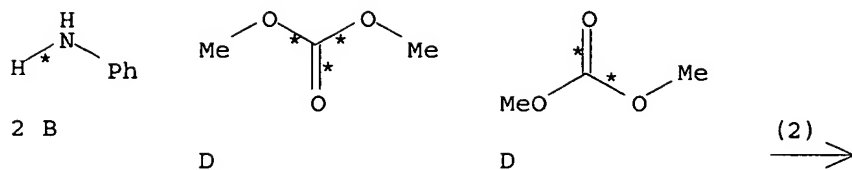
LANGUAGE: English

AB Mesoporous silica MCM-41, especially an Al-containing one, showed high
catalytic

activity for synthesis of phenylcarbamic acid Me ester from di-Me
carbonate and aniline at 363-383 K. It was easily separated from the product
solution, and the catalyst was able to be used repeatedly.

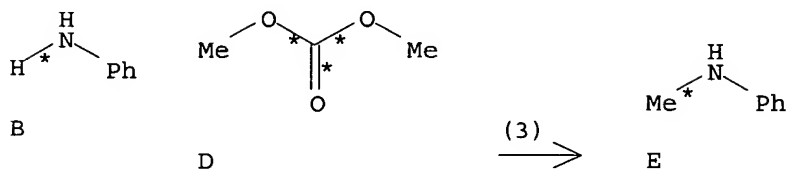
REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(2) OF 6 2 B + 2 D ==> C + E



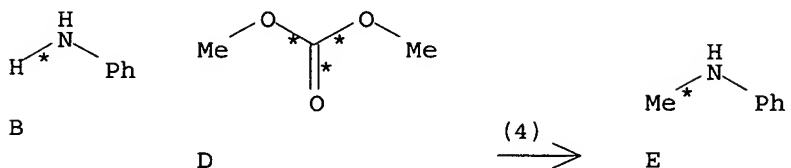
RX(2) RCT B 62-53-3, D 616-38-6
 PRO C 2603-10-3, E 100-61-8
 CAT 7631-86-9D SiO2

RX(3) OF 6 B + D ==> E



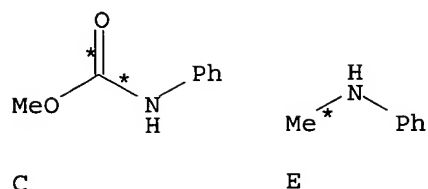
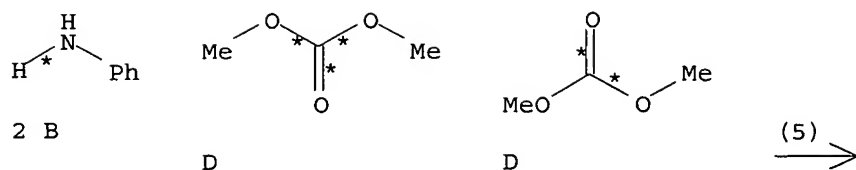
RX(3) RCT B 62-53-3, D 616-38-6
 PRO E 100-61-8
 CAT 7631-86-9D SiO2

RX(4) OF 6 B + D ==> E



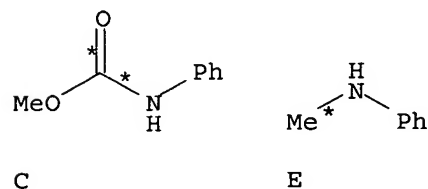
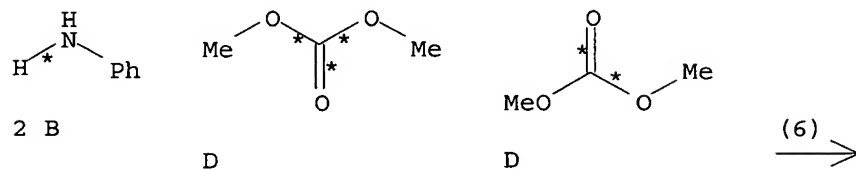
RX(4) RCT B 62-53-3, D 616-38-6
 PRO E 100-61-8
 CAT 7631-86-9D SiO2

RX(5) OF 6 2 B + 2 D ==> C + E



RX (5) RCT B 62-53-3, D 616-38-6
 PRO C 2603-10-3, E 100-61-8
 CAT 7631-86-9D SiO₂

RX (6) OF 6 2 B + 2 D ==> C + E



RX (6) RCT B 62-53-3, D 616-38-6
 PRO C 2603-10-3, E 100-61-8
 CAT 7631-86-9D SiO₂

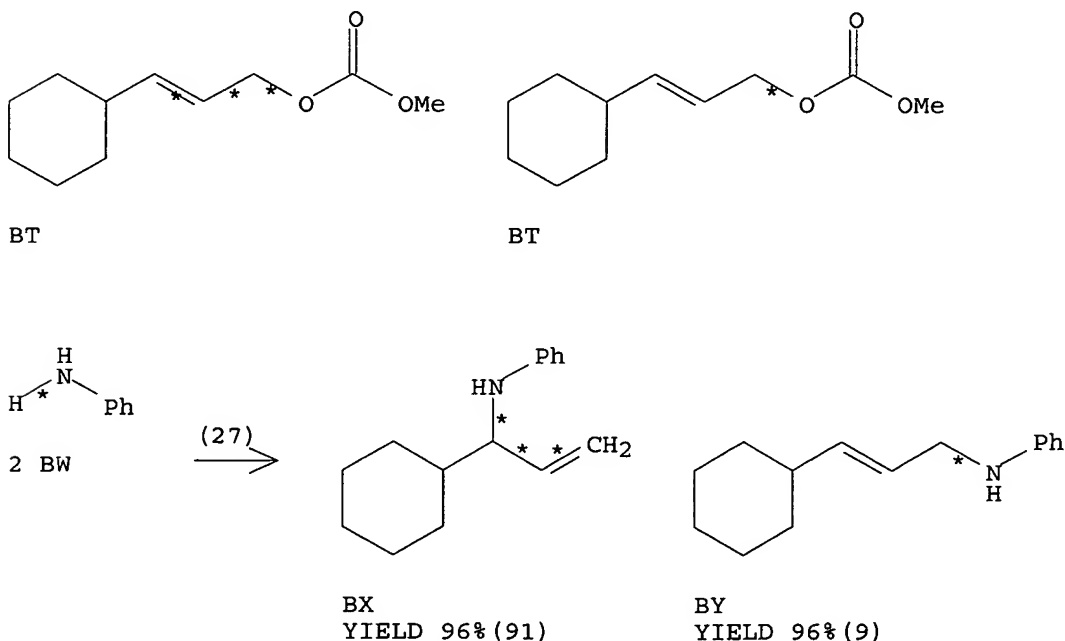
L60 ANSWER 27 OF 44 CASREACT COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 135:357537 CASREACT
 TITLE: Iridium complex-catalyzed allylic amination of allylic esters
 AUTHOR(S): Takeuchi, Ryo; Ue, Naoki; Tanabe, Keisuke; Yamashita, Kengo; Shiga, Norihito
 CORPORATE SOURCE: Department of Chemistry Graduate School of Integrated Science, Yokohama City University, Kanazawa-ku Yokohama, 236-0027, Japan

SOURCE: Journal of the American Chemical Society (2001),
123(39), 9525-9534
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Iridium complex-catalyzed allylic amination of allylic carbonates was studied. The solvent strongly affected the catalytic activity. The use of a polar solvent such as EtOH is essential for obtaining the products in high yield. The reaction of (E)-3-substituted-2-propenyl carbonate and 1-substituted-2-propenyl carbonate with pyrrolidine in the presence of a catalytic amount of [Ir(COD)Cl]₂ and P(OPh)₃ (P/Ir = 2) gave a branched amine with up to 99% selectivity. Both secondary and primary amines could be used for this reaction. When a primary amine was used, selective monoallylation occurred. No diallylation product was obtained. The reaction of 1,1-disubstituted-2-propenyl acetate H₂C:CHCR₁(OAc)Me (R₁ = n-pentyl, Me₂C:CHCH₂CH₂) with amines exclusively gave an α,α-disubstituted allylic amine H₂C:CHCR₁(NR₂)Me (NR₂ = piperidino, pyrrolidino, n-butylamino, anilino). This reaction provides an alternative route to the addition of an organometallic reagent to ketimines for the preparation of such amines. The reaction of (Z)-3-substituted-2-propenyl carbonate with amines gave (Z)-linear amines with up to 100% selectivity. In all cases, no (E)-linear amine was obtained. The selectivities described here have not been achieved in similar palladium complex-catalyzed reactions.

REFERENCE COUNT: 120 THERE ARE 120 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE REFORMAT

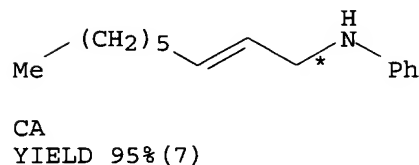
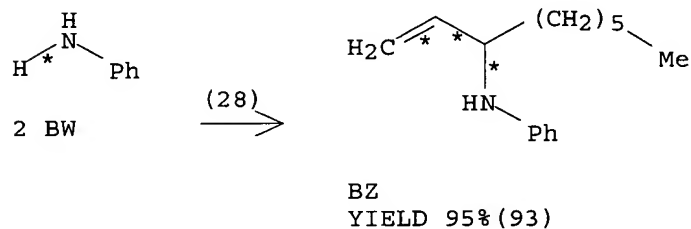
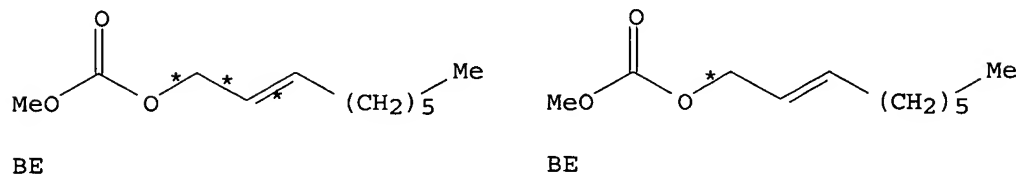
RX(27) OF 45 2 BT + 2 BW ==> BX + BY



RX(27) RCT BT 373362-32-4, BW 62-53-3
PRO BX 373362-42-6, BY 373362-49-3

CAT 101-02-0 P(OPh)₃, 12148-71-9 Iridium, bis[(1,2,5,6-η)-1,5-cyclooctadiene]di-μ-methoxydi-
 SOL 64-17-5 EtOH
 NTE optimization study, optimized on catalyst and solvent, regioselective, stereoselective

RX(28) OF 45 2 BE + 2 BW ==> BZ + CA



RX(28) RCT BE 373362-30-2, BW 62-53-3
 PRO BZ 373362-43-7, CA 373362-47-1
 CAT 101-02-0 P(OPh)₃, 12148-71-9 Iridium, bis[(1,2,5,6-η)-1,5-cyclooctadiene]di-μ-methoxydi-
 SOL 64-17-5 EtOH
 NTE optimization study, optimized on catalyst and solvent, regioselective, stereoselective

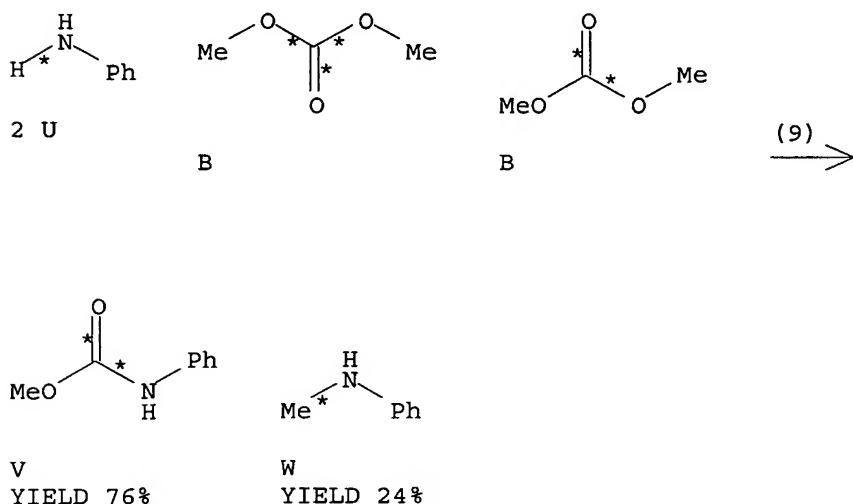
L60 ANSWER 28 OF 44 CASREACT COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 136:118057 CASREACT
 TITLE: 1,8-Diazabicyclo[5.4.0]undec-7-ene (DBU) and Microwave-Accelerated Green Chemistry in Methylation of Phenols, Indoles, and Benzimidazoles with Dimethyl Carbonate
 AUTHOR(S): Shieh, Wen-Chung; Dell, Steven; Repic, Oljan
 CORPORATE SOURCE: Chemical and Analytical Development, Novartis Institute for Biomedical Research, East Hanover, NJ, 07936, USA
 SOURCE: Organic Letters (2001), 3(26), 4279-4281
 CODEN: ORLEF7; ISSN: 1523-7060

PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB 1,8-Diazabicyclo[5.4.0]undec-7-ene (DBU) is a novel and active catalyst in promoting the methylation reaction of phenols, indoles, and benzimidazoles with di-Me carbonate under mild conditions. Addnl. rate enhancement is accomplished by applying microwave irradiation. By incorporating tetrabutylammonium iodide, the same microwave reactions can be further accelerated. By combining these acceleration strategies, very slow chemical transformations that take up to several days can be performed efficiently in high yield within minutes.

REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(9) OF 9 2 U + 2 B ==> V + W



RX(9) RCT U 62-53-3, B 616-38-6
 PRO V 2603-10-3, W 100-61-8
 CAT 6674-22-2 DBU
 NTE thermal, green chem.-reactant

L60 ANSWER 29 OF 44 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 134:193254 CASREACT

TITLE: Design, Synthesis, and Biological Evaluation of a Series of Lavendustin A Analogues That Inhibit EGFR and Syk Tyrosine Kinases, as Well as Tubulin Polymerization

AUTHOR(S): Mu, Fanrong; Coffing, Stephanie L.; Riese, David J., II; Geahlen, Robert L.; Verdier-Pinard, Pascal; Hamel, Ernest; Johnson, Jill; Cushman, Mark

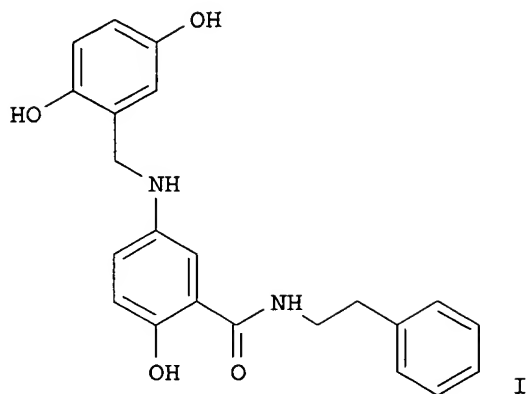
CORPORATE SOURCE: Department of Medicinal Chemistry and Molecular Pharmacology School of Pharmacy and Pharmacal Sciences, Purdue University, West Lafayette, IN, 47907, USA

SOURCE: Journal of Medicinal Chemistry (2001), 44(3), 441-452
 CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE:
LANGUAGE:
GI

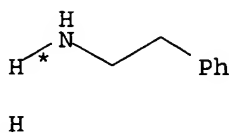
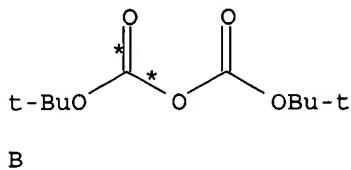
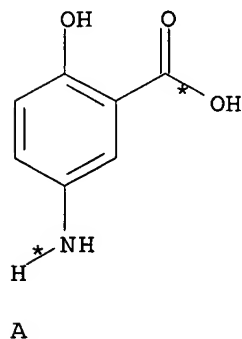
Journal
English

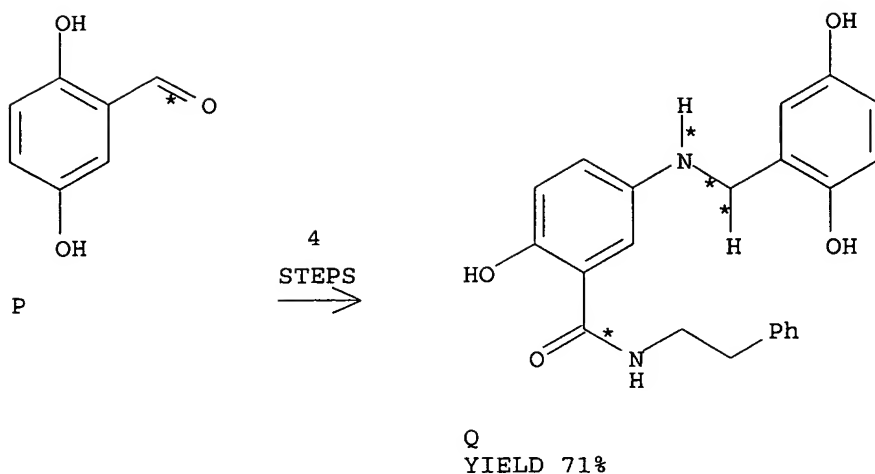


AB A series of N-alkylamide analogs of the lavendustin A pharmacophore, e.g. I, were synthesized and tested for inhibition of the epidermal growth factor receptor (EGFR) protein tyrosine kinase and the nonreceptor protein tyrosine kinase Syk. Although several compds. in the series were effective inhibitors of both kinases, it seemed questionable whether their inhibitory effects on these kinases were responsible for the cytotoxic properties observed in a variety of human cancer cell cultures. Accordingly, a COMPARE anal. of the cytotoxicity profile of the most cytotoxic member of the series was performed, and the results indicated that its cytotoxicity profile was similar to that of antitubulin agents. This mechanism of action was supported by demonstrating that most compds. in the series were moderately effective as inhibitors of tubulin polymerization. This suggests that the lavendustin A analogs reported here, as well as some of the previously reported lavendustin A analogs, may be acting as cytotoxic agents by a mechanism involving the inhibition of tubulin polymerization.

REFERENCE COUNT: 44 THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(120) OF 156 COMPOSED OF RX(1), RX(2), RX(3), RX(4)
RX(120) A + B + H + P ==> Q





RX(1) RCT A 89-57-6, B 24424-99-5

STAGE(1)

RGT D 121-44-8 Et3N

SOL 7732-18-5 Water, 123-91-1 Dioxane

STAGE(2)

RGT E 7647-01-0 HCl

SOL 7732-18-5 Water

PRO C 135321-95-8

RX(2) RCT C 135321-95-8

STAGE(1)

RGT D 121-44-8 Et3N, J 2592-95-2 1-Benzotriazolol, K 25952-53-8

EDAP

SOL 68-12-2 DMF

STAGE(2)

RCT H 64-04-0

STAGE(3)

SOL 7732-18-5 Water

PRO I 327037-08-1

RX(3) RCT I 327037-08-1

RGT N 76-05-1 F3CCO2H

PRO M 327037-09-2

SOL 75-09-2 CH2Cl2

RX(4) RCT M 327037-09-2, P 1194-98-5

STAGE(1)

SOL 71-43-2 Benzene

STAGE(2)

RGT R 25895-60-7 NaBH3CN

SOL 67-56-1 MeOH

STAGE(3)

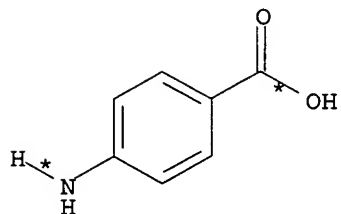
RGT E 7647-01-0 HCl, S 7647-14-5 NaCl

SOL 7732-18-5 Water

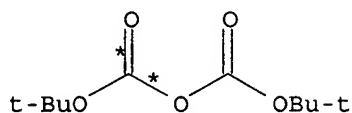
PRO Q 327037-10-5

RX(125) OF 156 COMPOSED OF RX(5), RX(6), RX(7), RX(8)

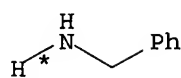
RX(125) V + B + X + P ==> AA



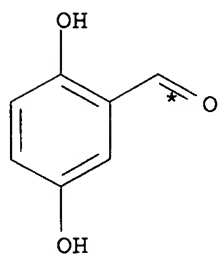
V



B

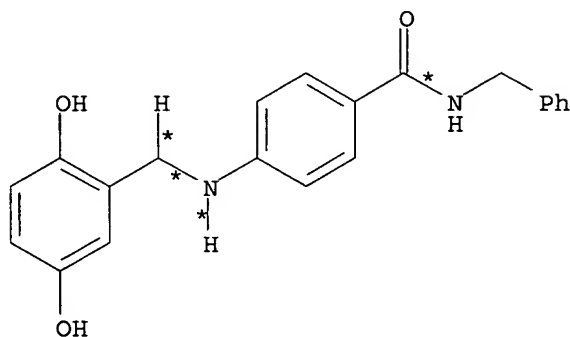


X



P

4
STEPS
→



AA
YIELD 77%

RX(5) RCT V 150-13-0, B 24424-99-5

STAGE(1)

RGT D 121-44-8 Et3N

SOL 7732-18-5 Water, 123-91-1 Dioxane

STAGE(2)

RGT E 7647-01-0 HCl

SOL 7732-18-5 Water

PRO W 66493-39-8

RX(6) RCT W 66493-39-8

STAGE(1)

RGT D 121-44-8 Et3N, J 2592-95-2 1-Benzotriazolol, K 25952-53-8

EDAP
SOL 68-12-2 DMF

STAGE(2)
RCT X 100-46-9

STAGE(3)
SOL 7732-18-5 Water

PRO Y 327037-11-6

RX(7) RCT Y 327037-11-6
RGT N 76-05-1 F3CCO2H
PRO Z 54977-92-3
SOL 75-09-2 CH2Cl2

RX(8) RCT P 1194-98-5, Z 54977-92-3

STAGE(1)
SOL 71-43-2 Benzene

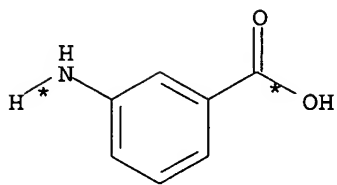
STAGE(2)
RGT R 25895-60-7 NaBH3CN
SOL 67-56-1 MeOH

STAGE(3)
RGT E 7647-01-0 HCl, S 7647-14-5 NaCl
SOL 7732-18-5 Water

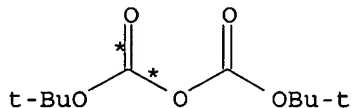
PRO AA 327037-12-7

RX(128) OF 156 COMPOSED OF RX(9), RX(10), RX(11), RX(12)

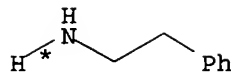
RX(128) AB + B + H + P ==> AF



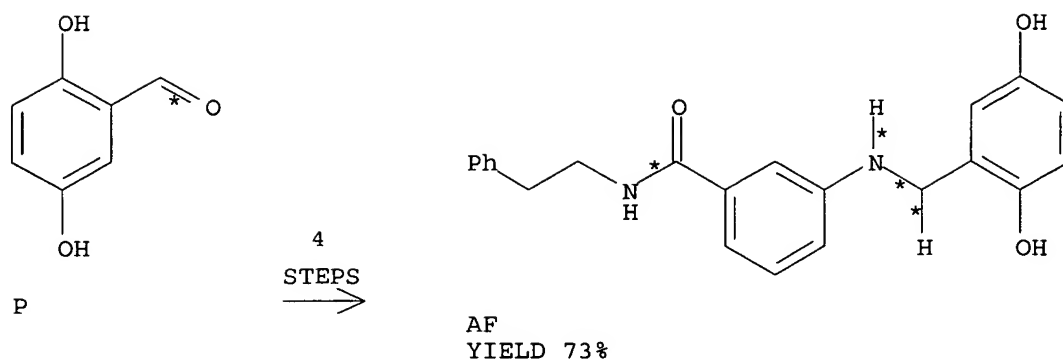
AB



B



H



RX(9) RCT AB 99-05-8, B 24424-99-5

STAGE(1)

RGT D 121-44-8 Et₃N

SOL 7732-18-5 Water, 123-91-1 Dioxane

STAGE(2)

RGT E 7647-01-0 HCl

SOL 7732-18-5 Water

PRO AC 111331-82-9

RX(10) RCT AC 111331-82-9

STAGE(1)

RGT D 121-44-8 Et₃N, J 2592-95-2 1-Benzotriazolol, K 25952-53-8
EDAP

SOL 68-12-2 DMF

STAGE(2)

RCT H 64-04-0

STAGE(3)

SOL 7732-18-5 Water

PRO AD 327037-14-9

RX(11) RCT AD 327037-14-9

RGT N 76-05-1 F₃CCO₂H

PRO AE 81882-72-6

SOL 75-09-2 CH₂Cl₂

RX(12) RCT P 1194-98-5, AE 81882-72-6

STAGE(1)

SOL 71-43-2 Benzene

STAGE(2)

RGT R 25895-60-7 NaBH₃CN

SOL 67-56-1 MeOH

STAGE(3)

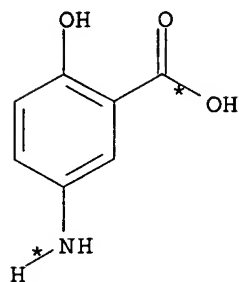
RGT E 7647-01-0 HCl, S 7647-14-5 NaCl

SOL 7732-18-5 Water

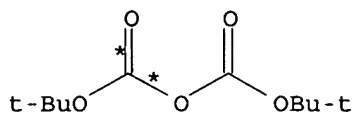
PRO AF 185019-03-8

RX(130) OF 156 COMPOSED OF RX(1), RX(13), RX(25), RX(37)

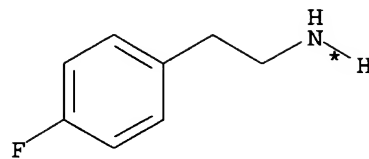
RX(130) A + B + AG + P ==> BP



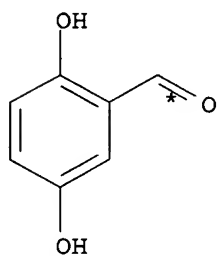
A



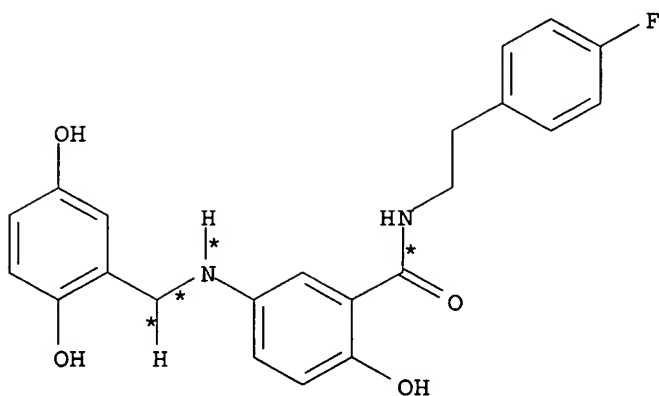
B



AG



P

4
STEPS
→BP
YIELD 42%

RX(1) RCT A 89-57-6, B 24424-99-5

STAGE(1)
RGT D 121-44-8 Et3N
SOL 7732-18-5 Water, 123-91-1 Dioxane

STAGE(2)
RGT E 7647-01-0 HCl
SOL 7732-18-5 Water

PRO C 135321-95-8

RX(13) RCT C 135321-95-8

STAGE(1)
RGT D 121-44-8 Et3N, J 2592-95-2 1-Benzotriazolol, K 25952-53-8
EDAP
SOL 68-12-2 DMF

STAGE(2)
RCT AG 1583-88-6

STAGE(3)
SOL 7732-18-5 Water

PRO AH 327037-15-0

RX(25) RCT AH 327037-15-0
RGT N 76-05-1 F3CCO2H
PRO BD 327037-27-4
SOL 75-09-2 CH2Cl2

RX(37) RCT P 1194-98-5, BD 327037-27-4

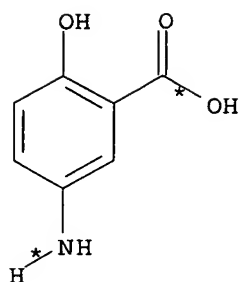
STAGE(1)
SOL 71-43-2 Benzene

STAGE(2)
RGT R 25895-60-7 NaBH3CN
SOL 67-56-1 MeOH

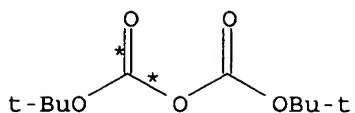
STAGE(3)
RGT E 7647-01-0 HCl, S 7647-14-5 NaCl
SOL 7732-18-5 Water

PRO BP 327037-38-7

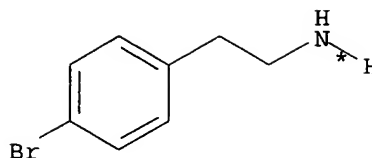
RX(132) OF 156 COMPOSED OF RX(1), RX(14), RX(26), RX(38)
RX(132) A + B + AI + P ==> BQ



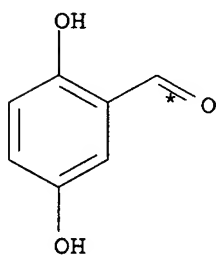
A



B

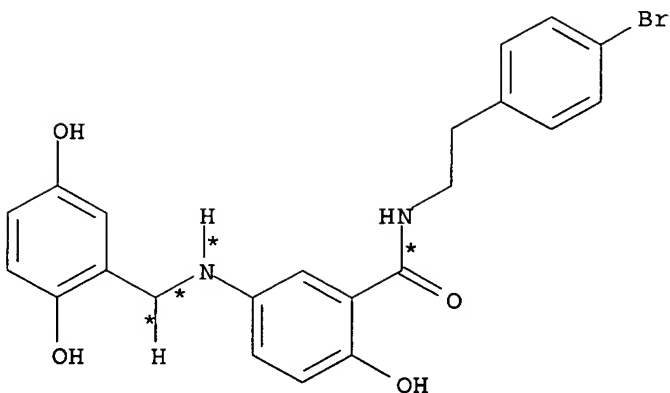


AI



P

4
STEPS
→



BQ

YIELD 64%

RX(1) RCT A 89-57-6, B 24424-99-5

STAGE(1)

RGT D 121-44-8 Et3N

SOL 7732-18-5 Water, 123-91-1 Dioxane

STAGE(2)

RGT E 7647-01-0 HCl

SOL 7732-18-5 Water

PRO C 135321-95-8

RX(14) RCT C 135321-95-8

STAGE(1)

RGT D 121-44-8 Et3N, J 2592-95-2 1-Benzotriazolol, K 25952-53-8
EDAP

SOL 68-12-2 DMF

STAGE(2)

RCT AI 73918-56-6

STAGE(3)

SOL 7732-18-5 Water

PRO AJ 327037-16-1

RX(26) RCT AJ 327037-16-1

RGT N 76-05-1 F3CCO2H

PRO BE 327037-28-5

SOL 75-09-2 CH2Cl2

RX(38) RCT P 1194-98-5, BE 327037-28-5

STAGE(1)

SOL 71-43-2 Benzene

STAGE(2)

RGT R 25895-60-7 NaBH3CN

SOL 67-56-1 MeOH

STAGE(3)

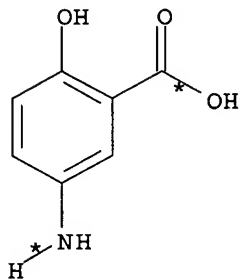
RGT E 7647-01-0 HCl, S 7647-14-5 NaCl

SOL 7732-18-5 Water

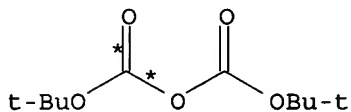
PRO BQ 327037-39-8

RX(134) OF 156 COMPOSED OF RX(1), RX(15), RX(27), RX(39)

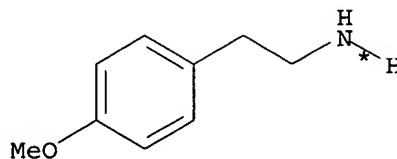
RX(134) A + B + AK + P ==> BR



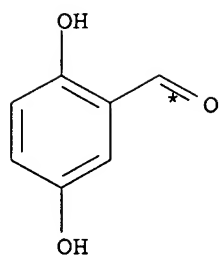
A



B

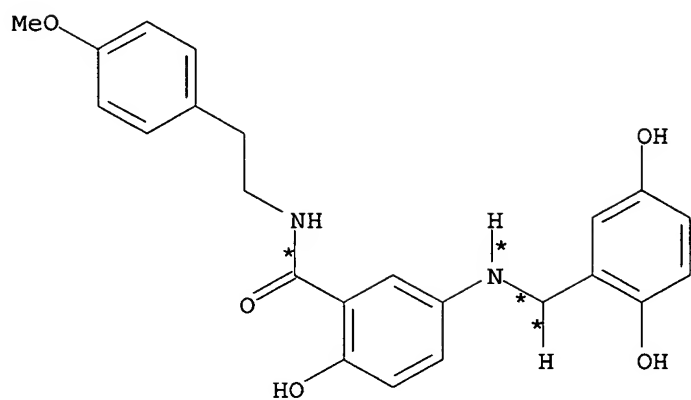


AK



P

4
STEPS
→



BR

YIELD 61%

RX(1) RCT A 89-57-6, B 24424-99-5

STAGE(1)

RGT D 121-44-8 Et3N

SOL 7732-18-5 Water, 123-91-1 Dioxane

STAGE(2)

RGT E 7647-01-0 HCl

SOL 7732-18-5 Water

PRO C 135321-95-8

RX(15) RCT C 135321-95-8

STAGE(1)

RGT D 121-44-8 Et3N, J 2592-95-2 1-Benzotriazolol, K 25952-53-8

EDAP

SOL 68-12-2 DMF

STAGE(2)

RCT AK 55-81-2

STAGE(3)

SOL 7732-18-5 Water

PRO AL 327037-17-2

RX(27) RCT AL 327037-17-2
RGT N 76-05-1 F3CCO2H
PRO BF 327037-29-6
SOL 75-09-2 CH2Cl2

RX(39) RCT P 1194-98-5, BF 327037-29-6

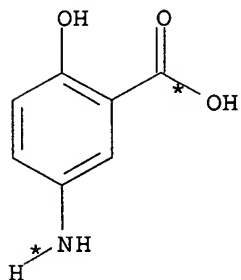
STAGE(1)
SOL 71-43-2 Benzene

STAGE(2)
RGT R 25895-60-7 NaBH3CN
SOL 67-56-1 MeOH

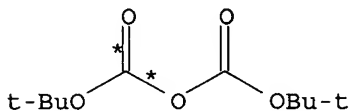
STAGE(3)
RGT E 7647-01-0 HCl, S 7647-14-5 NaCl
SOL 7732-18-5 Water

PRO BR 327037-40-1

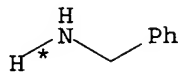
RX(136) OF 156 COMPOSED OF RX(1), RX(16), RX(28), RX(40)
RX(136) A + B + X + P ==> BS



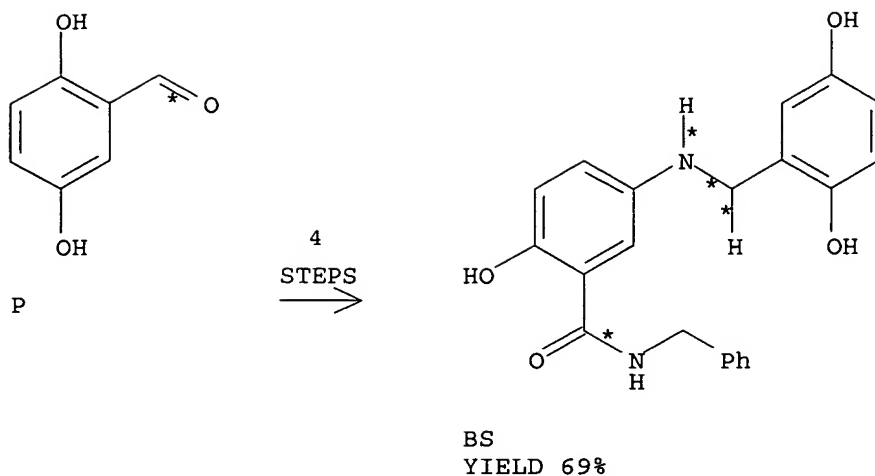
A



B



X



RX(1) RCT A 89-57-6, B 24424-99-5

STAGE(1)

RGT D 121-44-8 Et3N

SOL 7732-18-5 Water, 123-91-1 Dioxane

STAGE(2)

RGT E 7647-01-0 HCl

SOL 7732-18-5 Water

PRO C 135321-95-8

RX(16) RCT C 135321-95-8

STAGE(1)

RGT D 121-44-8 Et3N, J 2592-95-2 1-Benzotriazolol, K 25952-53-8

EDAP

SOL 68-12-2 DMF

STAGE(2)

RCT X 100-46-9

STAGE(3)

SOL 7732-18-5 Water

PRO AM 327037-18-3

RX(28) RCT AM 327037-18-3

RGT N 76-05-1 F3CCO2H

PRO BG 154737-59-4

SOL 75-09-2 CH2Cl2

RX(40) RCT P 1194-98-5, BG 154737-59-4

STAGE(1)

SOL 71-43-2 Benzene

STAGE(2)

RGT R 25895-60-7 NaBH3CN

SOL 67-56-1 MeOH

STAGE(3)

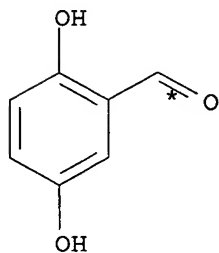
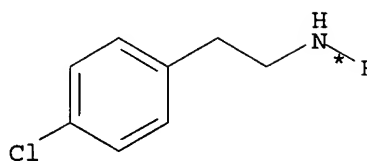
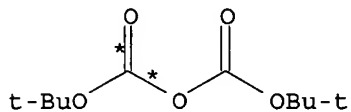
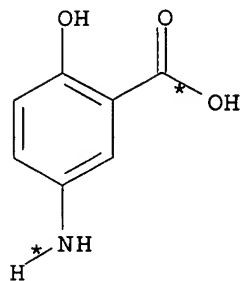
RGT E 7647-01-0 HCl, S 7647-14-5 NaCl

SOL 7732-18-5 Water

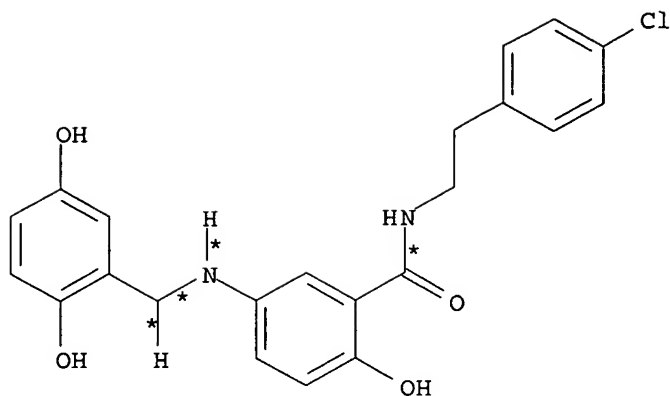
PRO BS 154736-69-3

RX(138) OF 156 COMPOSED OF RX(1), RX(17), RX(29), RX(41)

RX(138) A + B + AN + P ==> BT



4
STEPS
→



BT
YIELD 69%

RX(1) RCT A 89-57-6, B 24424-99-5

STAGE(1)

RGT D 121-44-8 Et3N

SOL 7732-18-5 Water, 123-91-1 Dioxane

STAGE(2)

RGT E 7647-01-0 HCl

SOL 7732-18-5 Water

PRO C 135321-95-8

RX(17) RCT C 135321-95-8

STAGE(1)

RGT D 121-44-8 Et3N, J 2592-95-2 1-Benzotriazolol, K 25952-53-8

EDAP

SOL 68-12-2 DMF

STAGE(2)

RCT AN 156-41-2

STAGE(3)

SOL 7732-18-5 Water

PRO AO 327037-19-4

RX(29) RCT AO 327037-19-4

RGT N 76-05-1 F3CCO2H

PRO BH 327037-30-9

SOL 75-09-2 CH2Cl2

RX(41) RCT P 1194-98-5, BH 327037-30-9

STAGE(1)

SOL 71-43-2 Benzene

STAGE(2)

RGT R 25895-60-7 NaBH3CN

SOL 67-56-1 MeOH

STAGE(3)

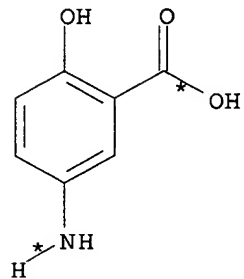
RGT E 7647-01-0 HCl, S 7647-14-5 NaCl

SOL 7732-18-5 Water

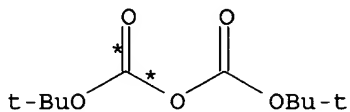
PRO BT 327037-41-2

RX(140) OF 156 COMPOSED OF RX(1), RX(18), RX(30), RX(42)

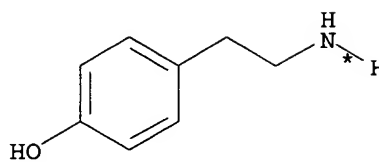
RX(140) A + B + AP + P ==> BU



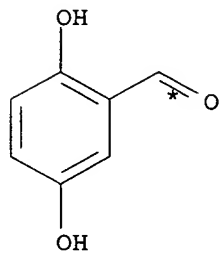
A



B

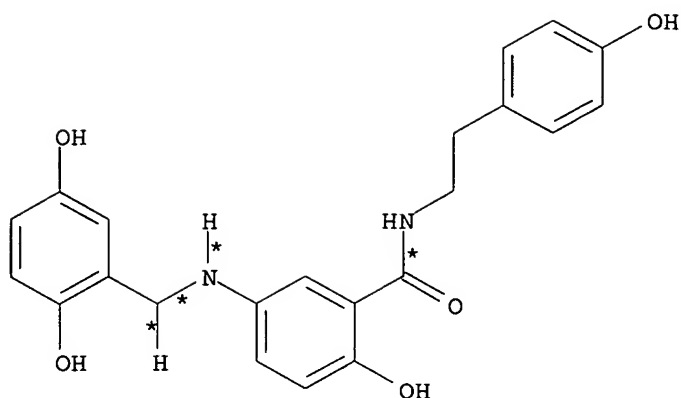


AP



P

4
STEPS
→



BU
YIELD 55%

RX(1) RCT A 89-57-6, B 24424-99-5

STAGE(1)

RGT D 121-44-8 Et3N

SOL 7732-18-5 Water, 123-91-1 Dioxane

STAGE(2)

RGT E 7647-01-0 HCl

SOL 7732-18-5 Water

PRO C 135321-95-8

RX(18) RCT C 135321-95-8

STAGE(1)

RGT D 121-44-8 Et3N, J 2592-95-2 1-Benzotriazolol, K 25952-53-8

EDAP

SOL 68-12-2 DMF

STAGE(2)

RCT AP 51-67-2

STAGE(3)

SOL 7732-18-5 Water

PRO AQ 327037-20-7

RX(30) RCT AQ 327037-20-7

RGT N 76-05-1 F3CCO2H

PRO BI 327037-31-0

SOL 75-09-2 CH2Cl2

RX(42) RCT P 1194-98-5, BI 327037-31-0

STAGE(1)

SOL 71-43-2 Benzene

STAGE(2)

RGT R 25895-60-7 NaBH3CN

SOL 67-56-1 MeOH

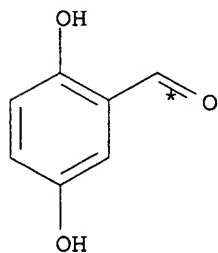
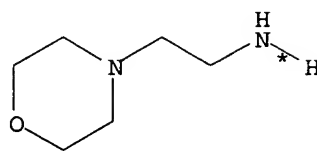
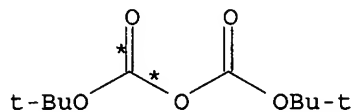
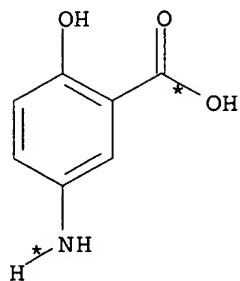
STAGE(3)

RGT E 7647-01-0 HCl, S 7647-14-5 NaCl

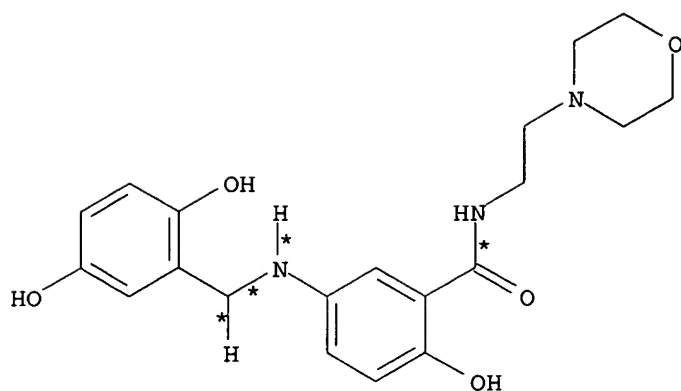
SOL 7732-18-5 Water

PRO BU 327037-42-3

RX(142) OF 156 COMPOSED OF RX(1), RX(19), RX(31), RX(43)
RX(142) A + B + AR + P ==> BV



4
STEPS
→



BV
YIELD 55%

RX(1) RCT A 89-57-6, B 24424-99-5

STAGE(1)

RGT D 121-44-8 Et3N

SOL 7732-18-5 Water, 123-91-1 Dioxane

STAGE(2)

RGT E 7647-01-0 HCl

SOL 7732-18-5 Water

PRO C 135321-95-8

RX(19) RCT C 135321-95-8

STAGE(1)

RGT D 121-44-8 Et3N, J 2592-95-2 1-Benzotriazolol, K 25952-53-8

EDAP

SOL 68-12-2 DMF

STAGE(2)

RCT AR 2038-03-1

STAGE(3)

SOL 7732-18-5 Water

PRO AS 327037-21-8

RX(31) RCT AS 327037-21-8

RGT N 76-05-1 F3CCO2H

PRO BJ 327037-32-1

SOL 75-09-2 CH2Cl2

RX(43) RCT P 1194-98-5, BJ 327037-32-1

STAGE(1)

SOL 71-43-2 Benzene

STAGE(2)

RGT R 25895-60-7 NaBH3CN

SOL 67-56-1 MeOH

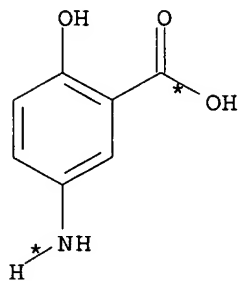
STAGE(3)

RGT E 7647-01-0 HCl, S 7647-14-5 NaCl

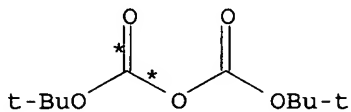
SOL 7732-18-5 Water

PRO BV 327037-43-4

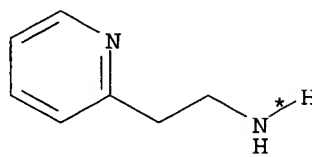
RX(144) OF 156 COMPOSED OF RX(1), RX(20), RX(32), RX(44)
RX(144) A + B + AT + P ==> BW



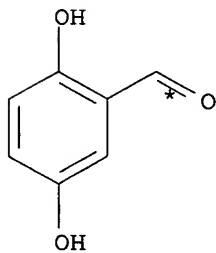
A



B

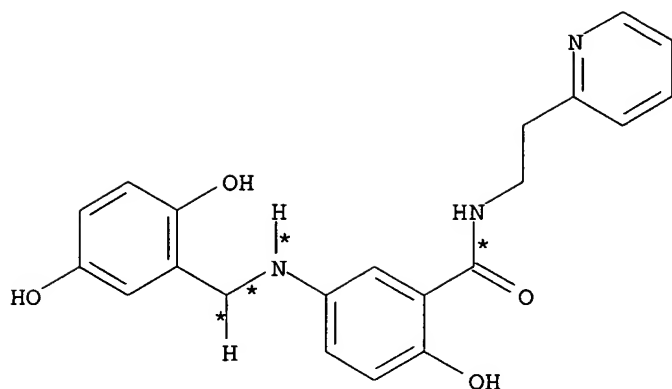


AT



P

4
STEPS
→



BW
YIELD 51%

RX(1) RCT A 89-57-6, B 24424-99-5

STAGE(1)

RGT D 121-44-8 Et3N

SOL 7732-18-5 Water, 123-91-1 Dioxane

STAGE(2)

RGT E 7647-01-0 HCl

SOL 7732-18-5 Water

PRO C 135321-95-8

RX(20) RCT C 135321-95-8

STAGE(1)

RGT D 121-44-8 Et3N, J 2592-95-2 1-Benzotriazolol, K 25952-53-8

EDAP

SOL 68-12-2 DMF

STAGE(2)

RCT AT 2706-56-1

STAGE(3)

SOL 7732-18-5 Water

PRO AU 327037-22-9

RX(32) RCT AU 327037-22-9

RGT N 76-05-1 F3CCO2H

PRO BK 327037-33-2

SOL 75-09-2 CH2Cl2

RX(44) RCT P 1194-98-5, BK 327037-33-2

STAGE(1)

SOL 71-43-2 Benzene

STAGE(2)

RGT R 25895-60-7 NaBH3CN

SOL 67-56-1 MeOH

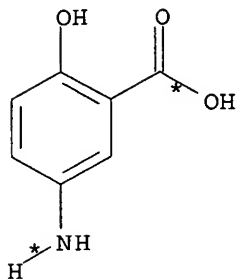
STAGE(3)

RGT E 7647-01-0 HCl, S 7647-14-5 NaCl

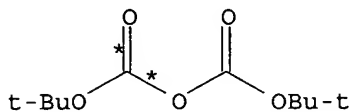
SOL 7732-18-5 Water

PRO BW 327037-44-5

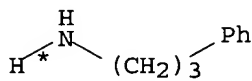
RX(146) OF 156 COMPOSED OF RX(1), RX(21), RX(33), RX(45)
 RX(146) A + B + AV + P ==> BX



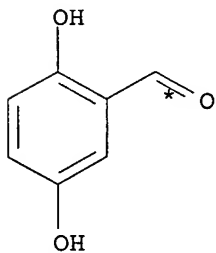
A



B

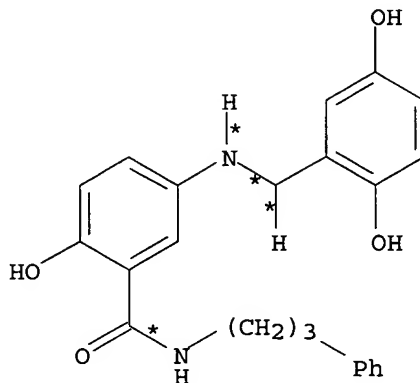


AV



P

4
STEPS
→



BX
YIELD 60%

RX(1) RCT A 89-57-6, B 24424-99-5

STAGE(1)

RGT D 121-44-8 Et3N

SOL 7732-18-5 Water, 123-91-1 Dioxane

STAGE(2)

RGT E 7647-01-0 HCl

SOL 7732-18-5 Water

PRO C 135321-95-8

RX(21) RCT C 135321-95-8

STAGE(1)

RGT D 121-44-8 Et3N, J 2592-95-2 1-Benzotriazolol, K 25952-53-8

EDAP

SOL 68-12-2 DMF

STAGE(2)

RCT AV 2038-57-5

STAGE(3)

SOL 7732-18-5 Water

PRO AW 327037-23-0

RX(33) RCT AW 327037-23-0

RGT N 76-05-1 F3CCO2H

PRO BL 327037-34-3

SOL 75-09-2 CH2Cl2

RX(45) RCT P 1194-98-5, BL 327037-34-3

STAGE(1)

SOL 71-43-2 Benzene

STAGE(2)

RGT R 25895-60-7 NaBH3CN

SOL 67-56-1 MeOH

STAGE(3)

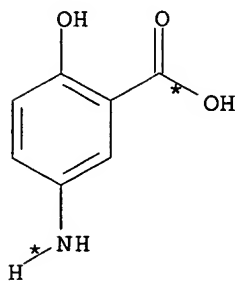
RGT E 7647-01-0 HCl, S 7647-14-5 NaCl

SOL 7732-18-5 Water

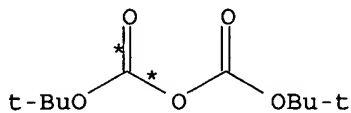
PRO BX 327037-45-6

RX(148) OF 156 COMPOSED OF RX(1), RX(22), RX(34), RX(46)

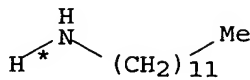
RX(148) A + B + AX + P ==> BY



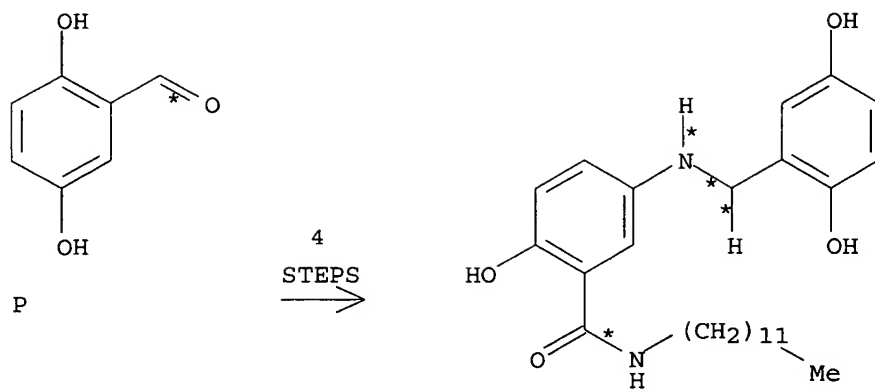
A



B



AX



BY
YIELD 56%

RX(1) RCT A 89-57-6, B 24424-99-5

STAGE(1)

RGT D 121-44-8 Et3N

SOL 7732-18-5 Water, 123-91-1 Dioxane

STAGE(2)

RGT E 7647-01-0 HCl

SOL 7732-18-5 Water

PRO C 135321-95-8

RX(22) RCT C 135321-95-8

STAGE(1)

RGT D 121-44-8 Et3N, J 2592-95-2 1-Benzotriazolol, K 25952-53-8

EDAP

SOL 68-12-2 DMF

STAGE(2)

RCT AX 124-22-1

STAGE(3)

SOL 7732-18-5 Water

PRO AY 327037-24-1

RX(34)

RCT AY 327037-24-1

RGT N 76-05-1 F3CCO2H

PRO BM 327037-35-4

SOL 75-09-2 CH2Cl2

RX(46)

RCT P 1194-98-5, BM 327037-35-4

STAGE(1)

SOL 71-43-2 Benzene

STAGE(2)

RGT R 25895-60-7 NaBH3CN

SOL 67-56-1 MeOH

STAGE(3)

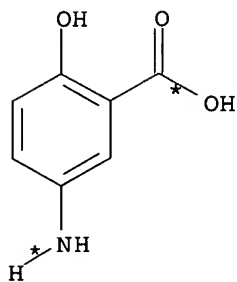
RGT E 7647-01-0 HCl, S 7647-14-5 NaCl

SOL 7732-18-5 Water

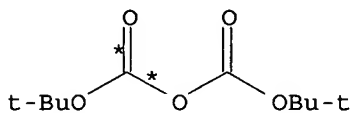
PRO BY 327037-46-7

RX(150) OF 156 COMPOSED OF RX(1), RX(23), RX(35), RX(47)

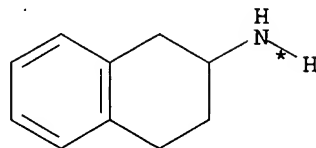
RX(150) A + B + AZ + P ==> BZ



A

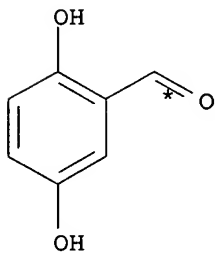


B

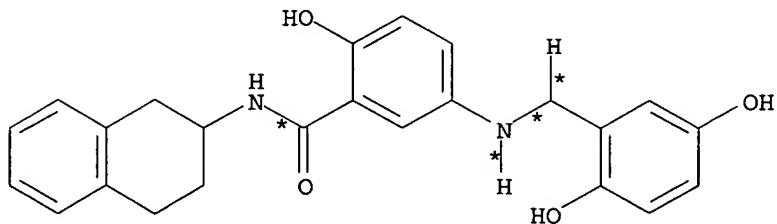


AZ

● HCl



P

4
STEPS
→

BZ

YIELD 61%

RX(1) RCT A 89-57-6, B 24424-99-5

STAGE(1)

RGT D 121-44-8 Et3N
SOL 7732-18-5 Water, 123-91-1 Dioxane

STAGE(2)

RGT E 7647-01-0 HCl
SOL 7732-18-5 Water

PRO C 135321-95-8

RX(23) RCT C 135321-95-8

STAGE(1)

RGT D 121-44-8 Et3N, J 2592-95-2 1-Benzotriazolol, K 25952-53-8
EDAP
SOL 68-12-2 DMF

STAGE(2)

RCT AZ 1743-01-7

STAGE(3)

SOL 7732-18-5 Water

PRO BA 327037-25-2

RX(35) RCT BA 327037-25-2
RGT N 76-05-1 F3CCO2H
PRO BN 327037-36-5
SOL 75-09-2 CH2Cl2

RX(47) RCT P 1194-98-5, BN 327037-36-5

STAGE(1)

SOL 71-43-2 Benzene

STAGE(2)

RGT R 25895-60-7 NaBH3CN
SOL 67-56-1 MeOH

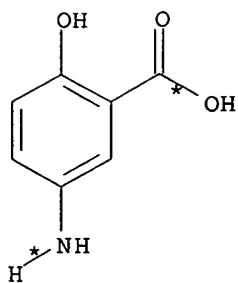
STAGE(3)

RGT E 7647-01-0 HCl, S 7647-14-5 NaCl
SOL 7732-18-5 Water

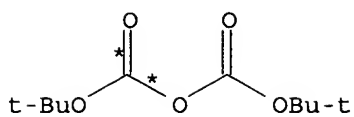
PRO BZ 327037-47-8

RX(152) OF 156 COMPOSED OF RX(1), RX(24), RX(36), RX(48)

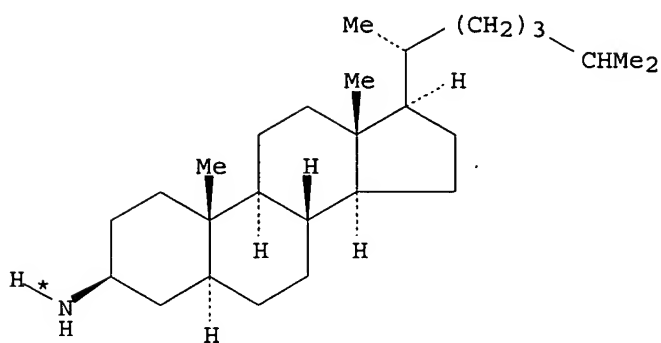
RX(152) A + B + BB + P ==> CA



A

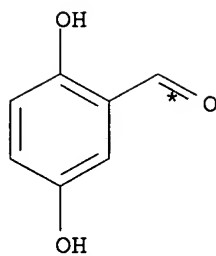


B



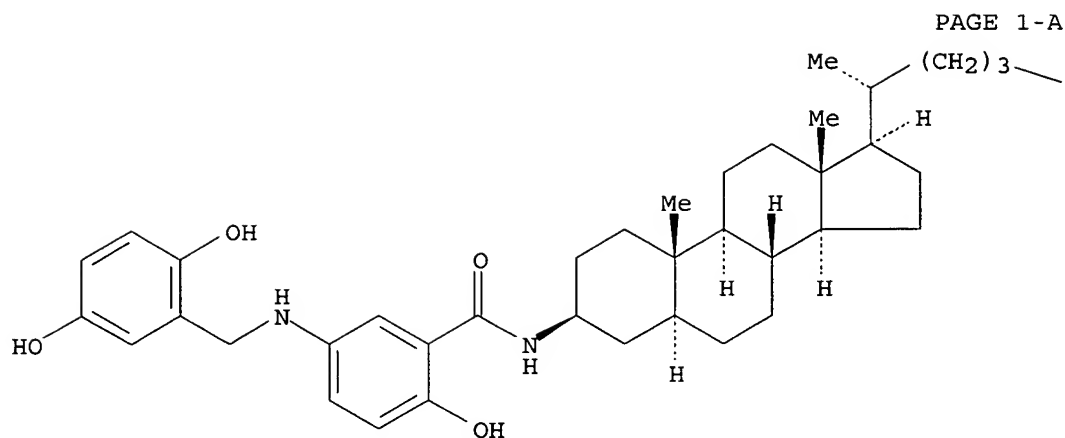
● HCl

BB



P

4
STEPS
→



CHMe₂

CA
YIELD 44%

RX(1) RCT A 89-57-6, B 24424-99-5

STAGE(1)

RGT D 121-44-8 Et₃N

SOL 7732-18-5 Water, 123-91-1 Dioxane

STAGE(2)

RGT E 7647-01-0 HCl

SOL 7732-18-5 Water

PRO C 135321-95-8

RX(24) RCT C 135321-95-8

STAGE(1)

RGT D 121-44-8 Et₃N, J 2592-95-2 1-Benzotriazolol, K 25952-53-8

EDAP

SOL 68-12-2 DMF

STAGE(2)

RCT BB 96290-48-1

STAGE(3)

SOL 7732-18-5 Water

PRO BC 327037-26-3

RX(36) RCT BC 327037-26-3
RGT N 76-05-1 F₃CCO₂H

PRO BO 327037-37-6
SOL 75-09-2 CH2Cl2

RX(48) RCT P 1194-98-5, BO 327037-37-6

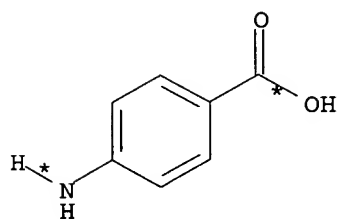
STAGE(1)
SOL 71-43-2 Benzene

STAGE(2)
RGT R 25895-60-7 NaBH3CN
SOL 67-56-1 MeOH

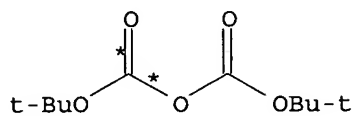
STAGE(3)
RGT E 7647-01-0 HCl, S 7647-14-5 NaCl
SOL 7732-18-5 Water

PRO CA 327037-48-9

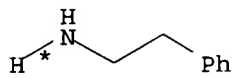
RX(154) OF 156 COMPOSED OF RX(5), RX(49), RX(51), RX(53)
RX(154) V + B + H + P ==> CF



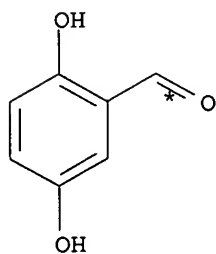
V



B

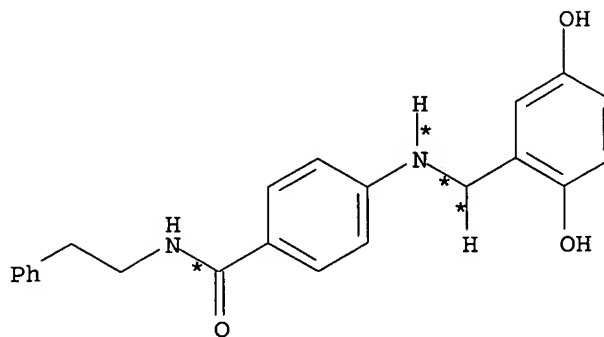


H



P

4
STEPS
=>



CF
YIELD 59%

RX(5) RCT V 150-13-0, B 24424-99-5

STAGE(1)
RGT D 121-44-8 Et3N
SOL 7732-18-5 Water, 123-91-1 Dioxane

STAGE(2)

RGT E 7647-01-0 HCl
SOL 7732-18-5 Water

PRO W 66493-39-8

RX(49) RCT W 66493-39-8

STAGE(1)

RGT D 121-44-8 Et3N, J 2592-95-2 1-Benzotriazolol, K 25952-53-8
EDAP
SOL 68-12-2 DMF

STAGE(2)

RCT H 64-04-0

STAGE(3)

SOL 7732-18-5 Water

PRO CB 327037-49-0

RX(51) RCT CB 327037-49-0
RGT N 76-05-1 F3CCO2H
PRO CD 61251-99-8
SOL 75-09-2 CH2Cl2

RX(53) RCT P 1194-98-5, CD 61251-99-8

STAGE(1)

SOL 71-43-2 Benzene

STAGE(2)

RGT R 25895-60-7 NaBH3CN
SOL 67-56-1 MeOH

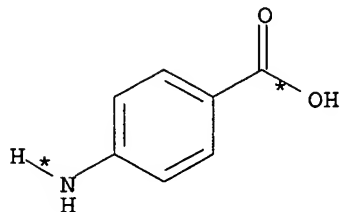
STAGE(3)

RGT E 7647-01-0 HCl, S 7647-14-5 NaCl
SOL 7732-18-5 Water

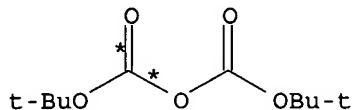
PRO CF 327037-52-5

RX(156) OF 156 COMPOSED OF RX(5), RX(50), RX(52), RX(54)

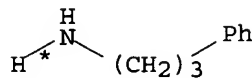
RX(156) V + B + AV + P ==> CG



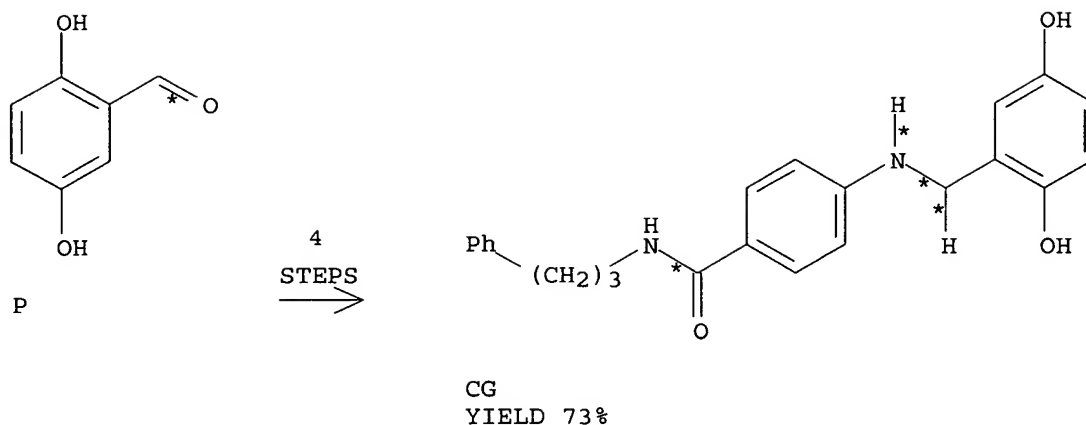
V



B



AV



RX(5) RCT V 150-13-0, B 24424-99-5

STAGE(1)

RGT D 121-44-8 Et3N

SOL 7732-18-5 Water, 123-91-1 Dioxane

STAGE(2)

RGT E 7647-01-0 HCl

SOL 7732-18-5 Water

PRO W 66493-39-8

RX(50) RCT W 66493-39-8

STAGE(1)

RGT D 121-44-8 Et3N, J 2592-95-2 1-Benzotriazolol, K 25952-53-8

EDAP

SOL 68-12-2 DMF

STAGE(2)

RCT AV 2038-57-5

STAGE(3)

SOL 7732-18-5 Water

PRO CC 327037-50-3

RX(52) RCT CC 327037-50-3

RGT N 76-05-1 F3CCO2H

PRO CE 327037-51-4

SOL 75-09-2 CH2Cl2

RX(54) RCT P 1194-98-5, CE 327037-51-4

STAGE(1)

SOL 71-43-2 Benzene

STAGE(2)

RGT R 25895-60-7 NaBH3CN

SOL 67-56-1 MeOH

STAGE(3)

RGT E 7647-01-0 HCl, S 7647-14-5 NaCl
SOL 7732-18-5 Water

PRO CG 327037-53-6

L60 ANSWER 30 OF 44 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 134:252292 CASREACT

TITLE: Carbonylation of o-Phenylenediamine and o-Aminophenol
with Dimethyl Carbonate Using Lead Compounds as
Catalysts

AUTHOR(S): Fu, Yue; Baba, Toshihide; Ono, Yoshio

CORPORATE SOURCE: Department of Chemical Engineering, Tokyo Institute of
Technology, Ookayama, Meguro-ku, Tokyo, 152-8552,
Japan

SOURCE: Journal of Catalysis (2001), 197(1), 91-97

CODEN: JCTLA5; ISSN: 0021-9517

PUBLISHER: Academic Press

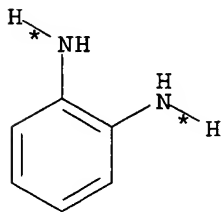
DOCUMENT TYPE: Journal

LANGUAGE: English

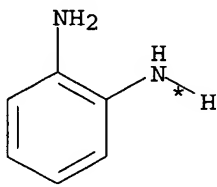
AB Lead compds. are active catalysts for carbonylation and
carbonylation/methylation of o-phenylenediamine and o-aminophenol with
di-Me carbonate (DMC). 2-Benzimidazolone was obtained in 84% yield by the
reaction of o-phenylenediamine with DMC for 1 h at 443 K in the presence
of Pb(NO₃)₂. In the presence of Pb(OAc)₂, the reaction quant. gave
1,3-dimethyl-2-benzimidazolone, which was formed by methylation of the
primary product, 2-benzimidazolone, at 473 K. The effects of reaction
variables on the yields of 2-benzimidazolone and 1,3-dimethyl-2-
benzimidazolone were examined. The reaction of o-aminophenol with DMC
selectively gave a carbonylation product, 2-benzoxazolone, or a
carbonylation/methylation product, 3-methyl-2-benzoxazolone, depending on
the reaction conditions in the presence of Pb(OAc)₂. (c) 2001 Academic
Press.

REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

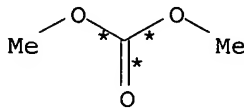
RX(1) OF 7 3 A + 3 B ==> C + D + E



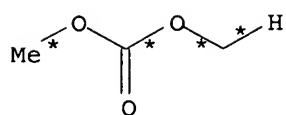
2 A



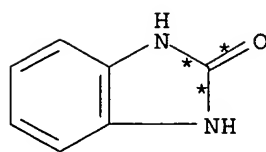
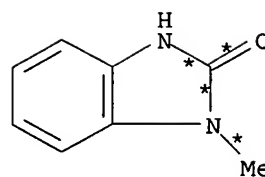
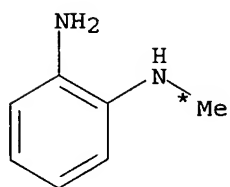
A



2 B

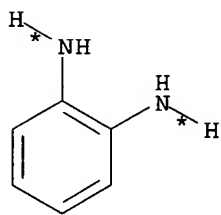


B

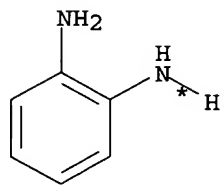
C
YIELD 77%D
YIELD 10%E
YIELD 13%

RX(1) RCT A 95-54-5, B 616-38-6
 PRO C 615-16-7, D 1849-01-0, E 4760-34-3
 CAT 10099-74-8 Pb(NO3)2
 NTE no solvent, alternative catalysts gave lower yields

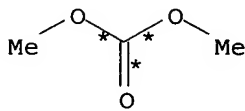
RX(5) OF 7 2 A + 2 B \implies C + E



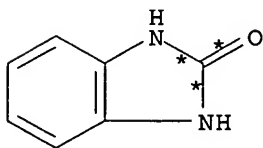
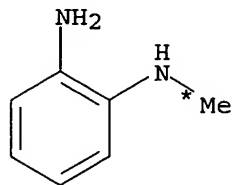
A



A

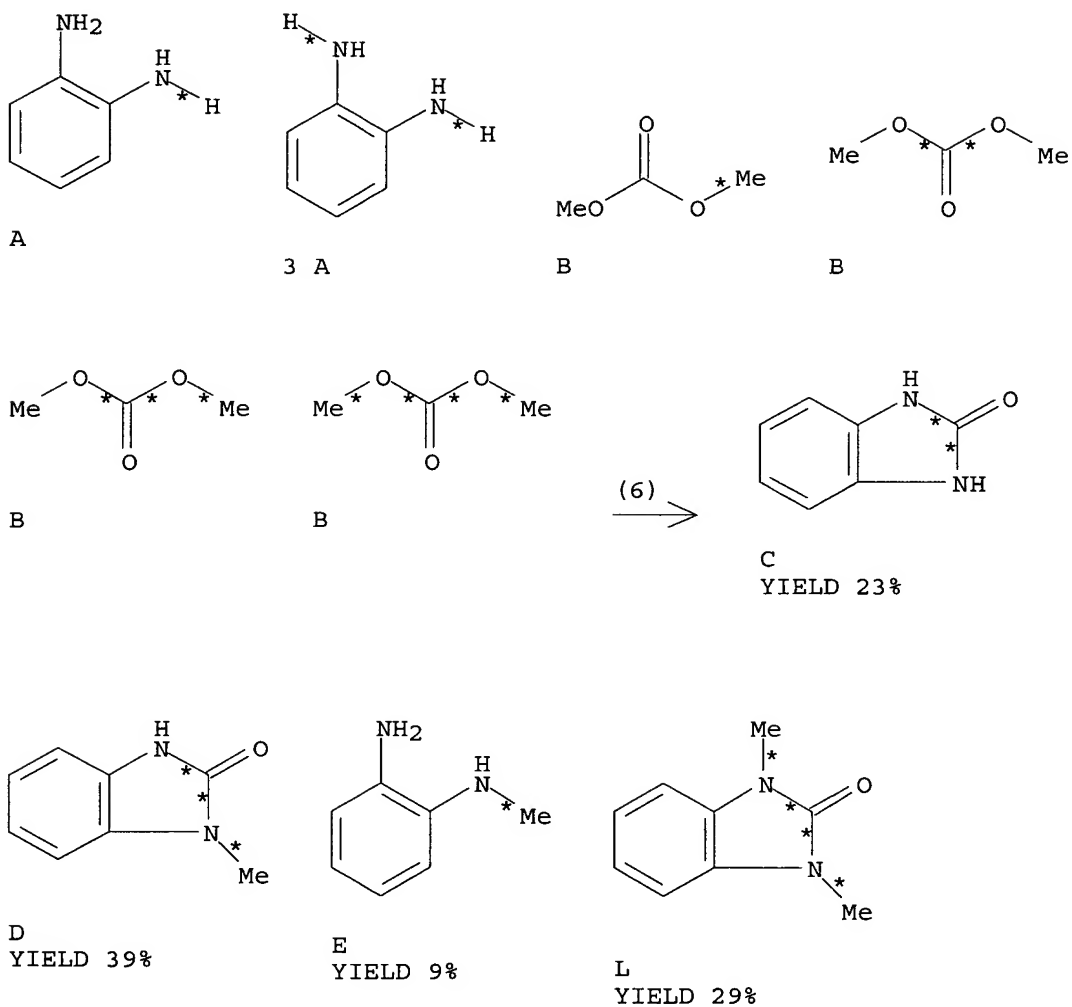


2 B

C
YIELD 5%E
YIELD 75%

RX(5) RCT A 95-54-5, B 616-38-6
 PRO C 615-16-7, E 4760-34-3
 NTE no solvent, use of catalysts gave lower yields

RX(6) OF 7 4 A + 4 B ==> C + D + E
 + L



RX(6) RCT A 95-54-5, B 616-38-6
 PRO C 615-16-7, D 1849-01-0, E 4760-34-3, L 3097-21-0
 CAT 10099-74-8 Pb(NO₃)₂
 NTE no solvent, alternative catalysts gave lower yields

L60 ANSWER 31 OF 44 CASREACT COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 132:207657 CASREACT
 TITLE: Preparation of linkers for solid phase synthesis
 INVENTOR(S): Nagai, Katsunori; Miwa, Tetsuo
 PATENT ASSIGNEE(S): Takeda Chemical Industries, Ltd., Japan

SOURCE: Eur. Pat. Appl., 42 pp.
 CODEN: EPXXDW
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 985662	A2	20000315	EP 1999-117080	19990831
EP 985662	A3	20030312		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
US 6388022	B1	20020514	US 1999-385953	19990830
CA 2281490	AA	20000310	CA 1999-2281490	19990909
CN 1247863	A	20000322	CN 1999-118556	19990909
KR 2000023020	A	20000425	KR 1999-38336	19990909
JP 2000143553	A2	20000523	JP 1999-255207	19990909
			JP 1998-257264	19980910

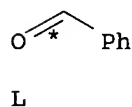
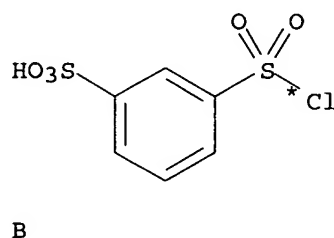
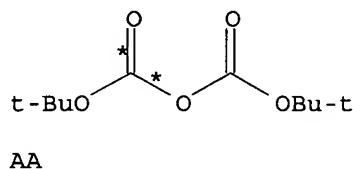
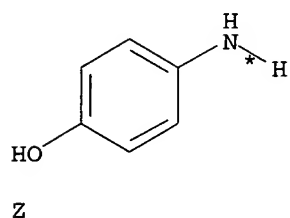
PRIORITY APPLN. INFO.:

OTHER SOURCE(S): MARPAT 132:207657

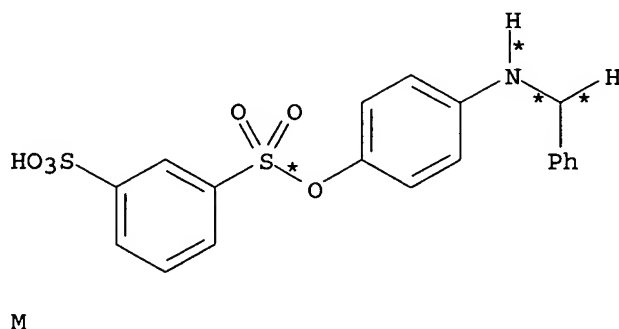
AB RYZW(SO₂X)_m [R = a carrier; X = leaving group; Y = bond or spacer; Z = bivalent electron-attracting group and W = (un)substituted di- or trivalent aromatic ring; Z = bivalent non-electron-attracting group and W = electron-attracting group-substituted aromatic ring; m = 1 or 2] were prepared and their use in solid phase synthesis demonstrated. Thus, 4-RC₆H₄SO₂C₆H₄(SO₂Cl)-3 (preparation given) was esterified by 4-(HO)C₆H₄NHCO₂CMe₃ and the deprotected product reductively alkylated by PhCHO to give 3-(4-RC₆H₄SO₂)C₆H₄SO₃C₆H₄(NHPh)-4 which was N-acylated by 3,4,5-trimethoxybenzoyl chloride and the product treated with Pd(OAc)₂/Ph₂P(CH₂)₃PPh₂/NEt₃/HCO₂H to give PhCH₂NPHCOC₆H₂(OMe)₃-3,4,5.

RX(21) OF 30 COMPOSED OF RX(7), RX(1), RX(3), RX(4)

RX(21) Z + AA + B + L ==> M



4
STEPS
→



RX(7) RCT Z 123-30-8, AA 24424-99-5
PRO A 54840-15-2
SOL 109-99-9 THF

RX(1) RCT A 54840-15-2, B 148344-35-8D
RGT D 121-44-8 Et3N
PRO C 260396-17-6D
SOL 109-99-9 THF
NTE RESIN SUPPORTED REACTION

RX(3) RCT C 260396-17-6D
RGT J 76-05-1 F3CCO2H
PRO I 260396-18-7D
SOL 75-09-2 CH2Cl2
NTE RESIN SUPPORTED REACTION

RX(4) RCT I 260396-18-7D, L 100-52-7

STAGE(1)
SOL 75-09-2 CH2Cl2

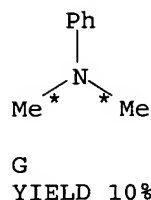
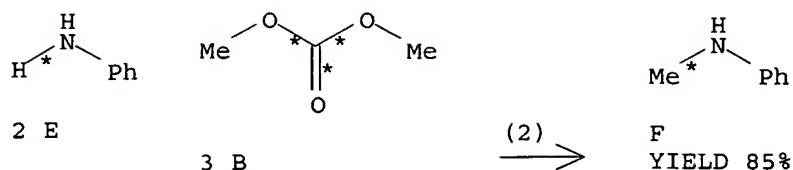
STAGE(2)
RGT N 64-19-7 AcOH, O 56553-60-7 Na.(AcO)3BH

STAGE(3)
SOL 68-12-2 DMF, 67-56-1 MeOH, 109-99-9 THF, 60-29-7 Et2O

PRO M 260396-19-8D
NTE RESIN SUPPORTED REACTION

L60 ANSWER 32 OF 44 CASREACT COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 134:4719 CASREACT
TITLE: Selective methylation of phenol, aniline and catechol
with dimethyl carbonate over calcined Mg-Al
hydrotalcites
AUTHOR(S): Jyothi, T. M.; Raja, T.; Talawar, M. B.; Sreekumar,
K.; Sugunan, S.; Rao, B. S.
CORPORATE SOURCE: National Chemical Laboratory, Pune, 411 021, India
SOURCE: Synthetic Communications (2000), 30(21), 3929-3934
CODEN: SYNCAV; ISSN: 0039-7911
PUBLISHER: Marcel Dekker, Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Calcined Mg-Al hydrotalcites (Mg/Al = 3) can be used as an efficient
catalyst in the selective O-methylation of phenol and catechol and
N-monomethylation of aniline employing (MeO)2CO as methylating agent in
vapor phase at 275°.
REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(2) OF 3 2 E + 3 B ==> F + G



RX(2) RCT E 62-53-3, B 616-38-6
 PRO F 100-61-8, G 121-69-7
 CAT 135752-28-2 Aluminum magnesium carbonate hydroxide
 NTE solid-support, silica

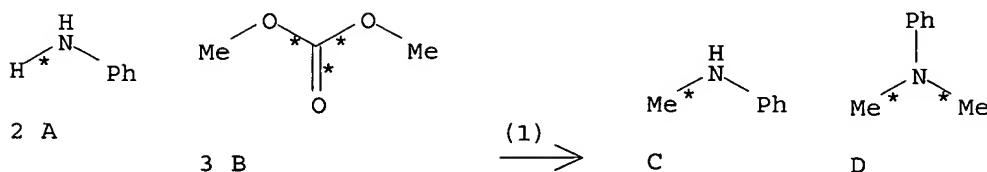
L60 ANSWER 33 OF 44 CASREACT COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 134:4715 CASREACT
 TITLE: Selective N-methylation of aniline with dimethyl carbonate over Zn_{1-x}CoxFe₂O₄ (x = 0, 0.2, 0.5, 0.8 and 1.0) type systems
 AUTHOR(S): Sreekumar, K.; Jyothi, T. M.; Mathew, T.; Talawar, M. B.; Sugunan, S.; Rao, B. S.
 CORPORATE SOURCE: Department of Applied Chemistry, Cochin University of Science and Technology, Cochin, 682 022, India
 SOURCE: Journal of Molecular Catalysis A: Chemical (2000), 159(2), 327-334
 CODEN: JMCCF2; ISSN: 1381-1169
 PUBLISHER: Elsevier Science B.V.
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB The alkylation of aniline with di-Me carbonate (DMC) is reported over Zn_{1-x}CoxFe₂O₄ (x = 0, 0.2, 0.5, 0.8 and 1.0) type systems prepared via. the copptn. route. The influence of surface acid-base properties, cation distribution in the spinel lattice and various reaction parameters are discussed. It was observed that systems possessing low x values are highly selective and active for N-alkylation leading to N-methylaniline as the major product. Since the authors have already reported the alkylation reaction using methanol as the alkylating agent over the same ferros spinel systems, in some cases the data are compared to highlight the merits and demerits of the choice of alkylating agent. DMC acts as a better alkylating agent at comparatively low temperature, where methanol shows only mild activity. However, on the selectivity basis DMC as an alkylating agent could not compete with methanol, since the former produced appreciable amount of N,N-dimethylaniline even at low temperature where methanol gave nearly 99% NMA selectivity. Cation distribution in the spinel lattice influences its acido-basic properties, and hence, these factors have been considered as helpful to evaluate the activity and stability of

the systems.

REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(1) OF 1 2 A + 3 B ==> C + D



RX(1) RCT A 62-53-3, B 616-38-6
 PRO C 100-61-8, D 121-69-7
 CAT 220942-91-6 Iron zinc oxide (Fe₃ZnO₄)
 NTE chemoselective, optimization study, catalyst compn. affects amt. of mono and di-N-alkylated products formed

L60 ANSWER 34 OF 44 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 133:207620 CASREACT

TITLE: A comparative study on aniline alkylation activity using methanol and dimethyl carbonate as the alkylating agents over Zn-Co-Fe ternary spinel systems
 AUTHOR(S): Sreekumar, K.; Mathew, T.; Mirajkar, S. P.; Sugunan, S.; Rao, B. S.

CORPORATE SOURCE: Department of Applied Chemistry, Cochin University of Science & Technology, Cochin, India

SOURCE: Applied Catalysis, A: General (2000), 201(1), L1-L8
 CODEN: ACAGE4; ISSN: 0926-860X

PUBLISHER: Elsevier Science B.V.

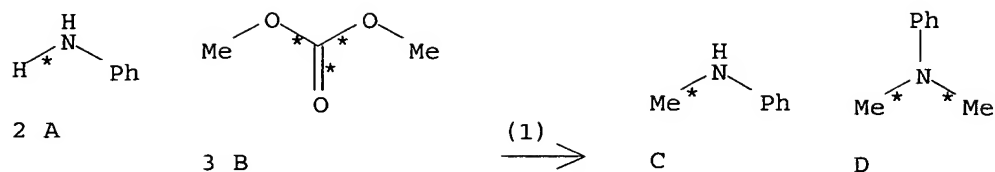
DOCUMENT TYPE: Journal

LANGUAGE: English

AB The catalyst compns. of the Zn_{1-x}Co_xFe₂O₄ (x= 0, 0.2, 0.5, 0.8 and 1.0) spinel series possessing 'x' values, x≤0.5, are unique for selective N-monomethylation of aniline using methanol as the alkylating agent. Catalysts thus prepared were Iron zinc oxide (Fe₂ZnO₄), cobalt iron zinc oxide (Co_{0.2}Fe₂Zn_{0.8}O₄), cobalt iron zinc oxide (Co_{0.5}Fe₂Zn_{0.5}O₄), cobalt iron zinc oxide (Co_{0.8}Fe₂Zn_{0.2}O₄), and cobalt iron oxide (CoFe₂O₄). Since di-Me carbonate (DMC) is another potential non-toxic alkylating agent, alkylation of aniline was investigated over various Zn-Co ferrites using DMC as the alkylating agent. The merits and demerits of the two alkylating agents are compared. Catalytic activity followed a similar trend with respect to the composition of the ferros spinel systems. DMC is active at comparatively low temperature, where methanol shows only mild activity. However, on the selectivity basis, DMC as an alkylating agent could not compete with methanol, since the former gave appreciable amts. of N,N-dimethylaniline (NNDMA) even at low temperature where methanol gave nearly 99% N-methylaniline (NMA) selectivity. As in the case of methanol, DMC also did not give any C-alkylated products.

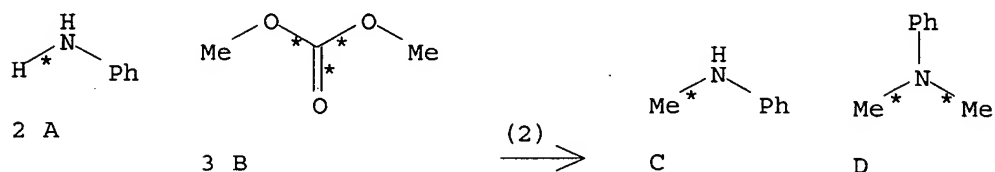
REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(1) OF 9 2 A + 3 B ==> C + D



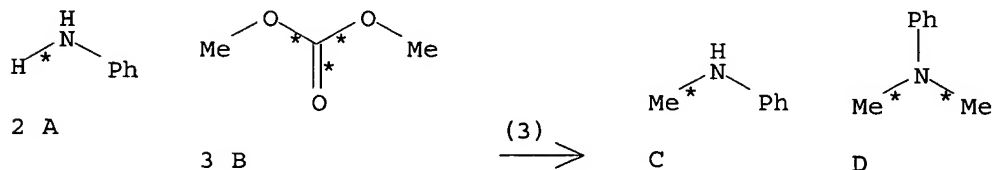
RX(1) RCT A 62-53-3, B 616-38-6
 PRO C 100-61-8, D 121-69-7
 CAT 12063-19-3 Iron zinc oxide (Fe₂ZnO₄)
 NTE vapor-phase down-flow silica reactor; (75.3:10.9 mono:di)

RX(2) OF 9 2 A + 3 B ==> C + D



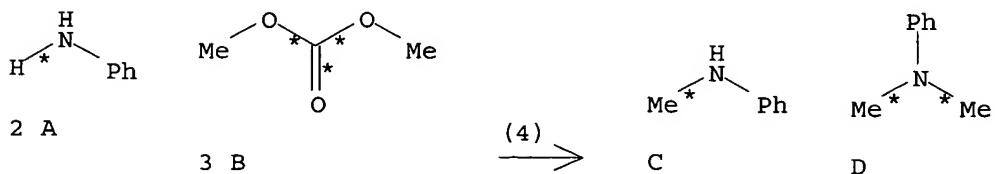
RX(2) RCT A 62-53-3, B 616-38-6
 PRO C 100-61-8, D 121-69-7
 CAT 118033-24-2 Cobalt iron zinc oxide (Co_{0.2}Fe₂Zn_{0.8}O₄)
 NTE vapor-phase down-flow silica reactor; (73.8:11.9 mono:di)

RX(3) OF 9 2 A + 3 B ==> C + D



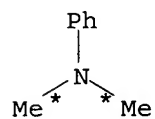
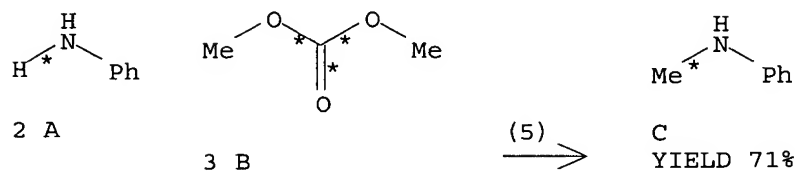
RX(3) RCT A 62-53-3, B 616-38-6
 PRO C 100-61-8, D 121-69-7
 CAT 111568-68-4 Cobalt iron zinc oxide (Co_{0.8}Fe₂Zn_{0.2}O₄)
 NTE vapor-phase down-flow silica reactor; (62.2:20.1 mono:di)

RX(4) OF 9 2 A + 3 B ==> C + D



RX(4) RCT A 62-53-3, B 616-38-6
 PRO C 100-61-8, D 121-69-7
 CAT 12052-28-7 Cobalt iron oxide (CoFe₂O₄)
 NTE vapor-phase down-flow silica reactor; (61.2:21.1 mono:di)

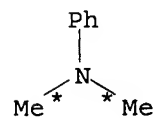
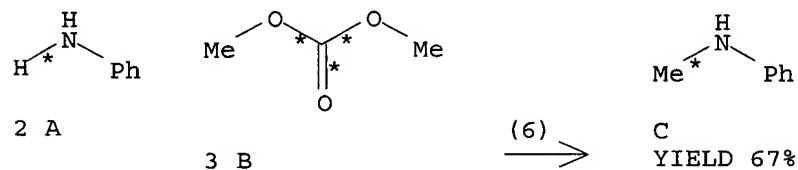
RX(5) OF 9 2 A + 3 B ==> C + D



D
 YIELD 7%

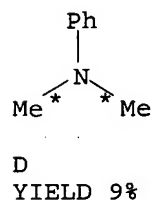
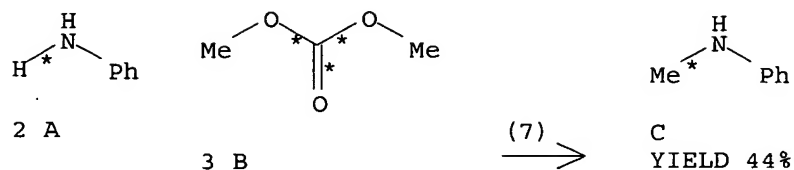
RX(5) RCT A 62-53-3, B 616-38-6
 PRO C 100-61-8, D 121-69-7
 CAT 12063-19-3 Iron zinc oxide (Fe₂ZnO₄)
 NTE vapor-phase down-flow silica reactor; yields vary with temp.

RX(6) OF 9 2 A + 3 B ==> C + D

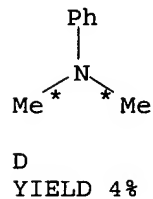
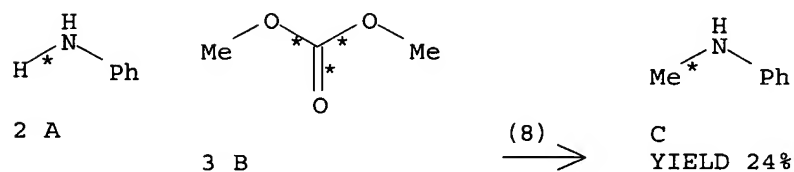


D
 YIELD 5%

RX(6) RCT A 62-53-3, B 616-38-6
 PRO C 100-61-8, D 121-69-7
 CAT 118033-24-2 Cobalt iron zinc oxide (Co_{0.2}Fe₂Zn_{0.8}O₄)

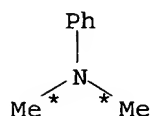
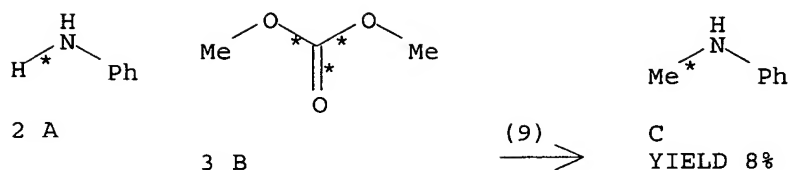
$$\text{RX (7) OF 9} \quad 2 \text{ A} + 3 \text{ B} \implies \text{C} + \text{D}$$


RX (7) RCT A 62-53-3, B 616-38-6
 PRO C 100-61-8, D 121-69-7
 CAT 111568-47-9 Cobalt iron zinc oxide (Co_{0.5}Fe₂Zn_{0.5}O₄)
 NTE vapor-phase down-flow silica reactor; yields vary with temp.

$$\text{RX (8) OF 9} \quad 2 \text{ A} + 3 \text{ B} \implies \text{C} + \text{D}$$


RX (8)	RCT	A 62-53-3, B 616-38-6
	PRO	C 100-61-8, D 121-69-7
	CAT	111568-68-4 Cobalt iron zinc oxide (Co _{0.8} Fe ₂ Zn _{0.2} O ₄)
	NTE	vapor-phase down-flow silica reactor; yields vary with temp.

$$\text{RX (9) OF 9} \quad 2 \text{ A} + 3 \text{ B} \implies \text{C} + \text{D}$$



D
YIELD 2%

RX(9) RCT A 62-53-3, B 616-38-6
 PRO C 100-61-8, D 121-69-7
 CAT 12052-28-7 Cobalt iron oxide (CoFe2O4)
 NTE vapor-phase down-flow silica reactor; yields vary with temp.

L60 ANSWER 35 OF 44 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 129:216469 CASREACT

TITLE: Ligand effects in the metal catalyzed reactions of
N-aryldiazoamides: ylide formation vs. insertion
reactions

AUTHOR(S): Moody, Christopher J.; Miah, Soyfur; Slawin, Alexandra
M. Z.; Mansfield, Darren J.; Richards, Ian C.

CORPORATE SOURCE: Dep. Chem., Loughborough Univ., Leicestershire, LE11
3TU, UK

SOURCE: Tetrahedron (1998), 54(33), 9689-9700

CODEN: TETRAB; ISSN: 0040-4020

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

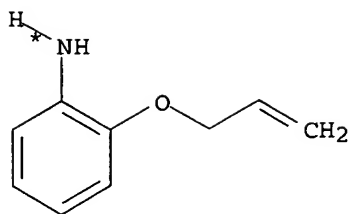
LANGUAGE: English

AB Diazoamides 2-CH₂:CHCH₂XC₆H₄N(CH₂Ph)COC(:N₂)CO₂Et (I, X = O, S) were prepared from 2-(O-allyl)- and 2-(S-allyl) anilines, resp. Copper(II) catalyzed decomposition of I resulted in formation of benzo-fused heterocycles by [2,3]-rearrangement of the intermediate ylide. Rhodium(II) perfluorobutyramide catalyzed reaction, however, gave mainly indoles; rhodium(II) acetate catalyzed reaction resulted in a mixture of products, with β-lactams formed by intramol. C-H insertion predominating. Catalyzed decomposition of a N-pyridyl diazoamide gave a stable pyridinium ylide.

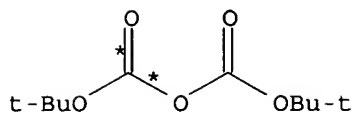
REFERENCE COUNT: 42 THERE ARE 42 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(34) OF 65 COMPOSED OF RX(1), RX(3), RX(5)

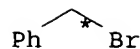
RX(34) A + B + G ==> M



A

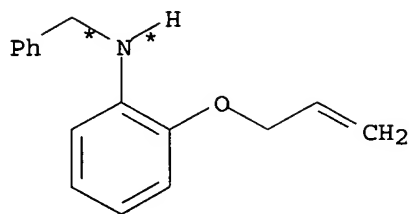


B



G

3
STEPS
→



M
YIELD 94%

RX(1) RCT A 27096-64-6, B 24424-99-5
PRO C 212475-56-4
SOL 109-99-9 THF

RX(3) RCT C 212475-56-4

STAGE(1)

RGT I 7646-69-7 NaH
SOL 68-12-2 DMF

STAGE(2)

RCT G 100-39-0

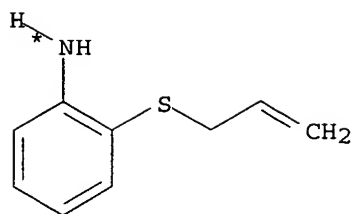
STAGE(3)

RGT J 7732-18-5 Water

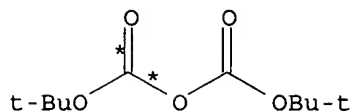
PRO H 212475-60-0

RX(5) RCT H 212475-60-0
RGT N 76-05-1 F3CCO2H
PRO M 212475-64-4
SOL 75-09-2 CH2Cl2

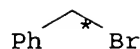
RX(35) OF 65 COMPOSED OF RX(2), RX(4), RX(6)
RX(35) E + B + G ==> P



E

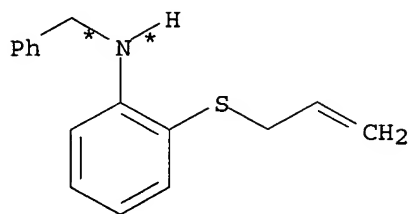


B



G

3
STEPS
→



P
YIELD 99%

RX(2) RCT E 77053-20-4, B 24424-99-5
PRO F 212475-58-6
SOL 109-99-9 THF

RX(4) RCT F 212475-58-6

STAGE(1)

RGT I 7646-69-7 NaH
SOL 68-12-2 DMF

STAGE(2)

RCT G 100-39-0

STAGE(3)

RGT J 7732-18-5 Water

PRO L 212475-62-2

RX(6) RCT L 212475-62-2
RGT N 76-05-1 F3CCO2H
PRO P 212475-66-6
SOL 75-09-2 CH2Cl2

L60 ANSWER 36 OF 44 CASREACT COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 123:228227 CASREACT

TITLE: Preparation of 1-acylmethyl-2-oxo-3-phenylureido-5-heterocyclyl-1,4-benzodiazepines useful as CCK-B and/or gastrin receptor antagonists.

INVENTOR(S): Semple, Graeme; Ryder, Hamish; Szelke, Michael; Satoh, Masato; Ohta, Mitsuaki; Miyata, Keiji; Nishida, Akito; Ishii, Masato

PATENT ASSIGNEE(S): Yamanouchi Pharmaceutical Co. Ltd., Japan; Ferring Research Ltd.

SOURCE: PCT Int. Appl., 77 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

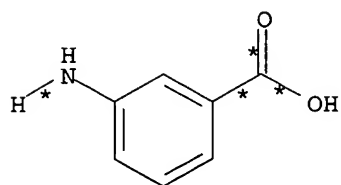
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9506040	A1	19950302	WO 1994-GB1859	19940825
W: AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, JP, KE, KG, KP, KR, KZ, LK, LT, LU, LV, MD, MG, MN, MW, NL, NO, NZ, PL, PT, RO, RU, SD, SE, SI, SK, TJ, TT, UA, US, UZ, VN				
RW: KE, MW, SD, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
GB 2282595	A1	19950412	GB 1993-17693	19930825
CA 2169089	AA	19950302	CA 1994-2169089	19940825
AU 9474661	A1	19950321	AU 1994-74661	19940825
AU 687433	B2	19980226		
ZA 9406474	A	19960325	ZA 1994-6474	19940825
EP 715624	A1	19960612	EP 1994-924368	19940825
EP 715624	B1	19980408		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
CN 1129442	A	19960821	CN 1994-193134	19940825
HU 73978	A2	19961028	HU 1996-205	19940825
JP 09504005	T2	19970422	JP 1994-507439	19940825
AT 164840	E	19980415	AT 1994-924368	19940825
ES 2117797	T3	19980816	ES 1994-924368	19940825
FI 9600836	A	19960422	FI 1996-836	19960223
NO 9600747	A	19960425	NO 1996-747	19960223
✓ US 5728829	A	19980317	US 1996-591567	19960502
PRIORITY APPLN. INFO.:			GB 1993-17693	19930825
			WO 1994-GB1859	19940825
OTHER SOURCE(S):			MARPAT 123:228227	
GI				

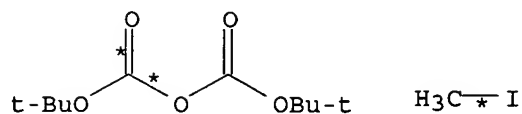
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Title compds. [I; R4 = alkyl, cycloalkyl, aryl; R10 = halo, OH, Me, OMe, NR11R12, NO2, NHCHO, CO2H, cyano; R11, R12 = H, alkyl; NR11R12 = Q1; a = 1-6; R2 = aromatic 5- or 6-membered (substituted) heterocyclyl containing ≥2 heteroatoms of which ≥1 is N], were prepared Thus, title compound (II), prepared from 2-aminophenyl 2-thiazolyl ketone via 3-amino-1-tert-butylcarbonylmethyl-2,3-dihydro-5-(2-thiazolyl)-1H-1,4-benzodiazepin-2-one, at 0.1 μmol/kg in rats inhibited pentagastrin-stimulated gastric acid secretion by 55.2%. Tablets were prepared containing II.

RX(284) OF 419 COMPOSED OF RX(73), RX(84), RX(85), RX(22)
 RX(284) **CY** + **EQ** + EP + AI ==> **BD**

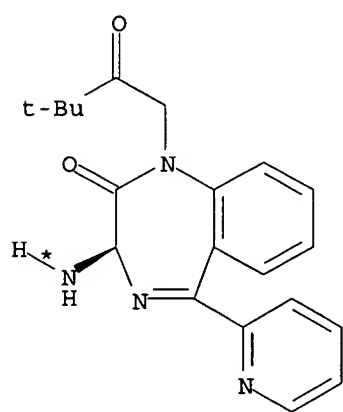


CY



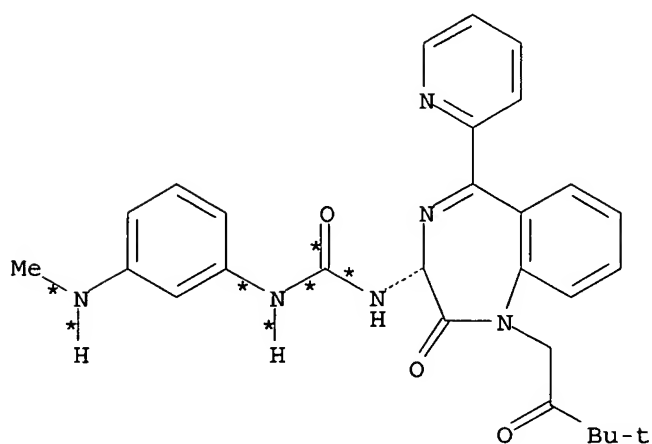
EQ

EP



AI

4
 STEPS
 →



BD
 YIELD 72%

RX(73) RCT CY 99-05-8

STAGE(1)

RGT CD 1310-58-3 KOH

SOL 123-91-1 Dioxane, 7732-18-5 Water

STAGE(2)

RCT EQ 24424-99-5

PRO AR 111331-82-9

RX(84) RCT AR 111331-82-9

STAGE(1)

RGT BQ 7646-69-7 NaH

SOL 68-12-2 DMF

STAGE(2)

RCT EP 74-88-4

STAGE(3)

RGT FN 1310-65-2 LiOH

SOL 67-56-1 MeOH

STAGE(4)

RGT U 7647-01-0 HCl

SOL 7732-18-5 Water

PRO FM 168162-30-9

RX(85) RCT FM 168162-30-9

STAGE(1)

RGT G 121-44-8 Et3N, EK 541-41-3 ClCO2Et

SOL 67-64-1 Me2CO

STAGE(2)

RGT EL 26628-22-8 NaN3

SOL 7732-18-5 Water

PRO BC 168162-32-1

RX(22) RCT BC 168162-32-1, AI 164343-31-1

STAGE(1)

SOL 75-09-2 CH2Cl2

STAGE(2)

RGT U 7647-01-0 HCl

SOL 7732-18-5 Water

STAGE(3)

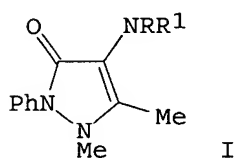
RGT O 1310-73-2 NaOH

SOL 7732-18-5 Water

PRO BD 155488-25-8

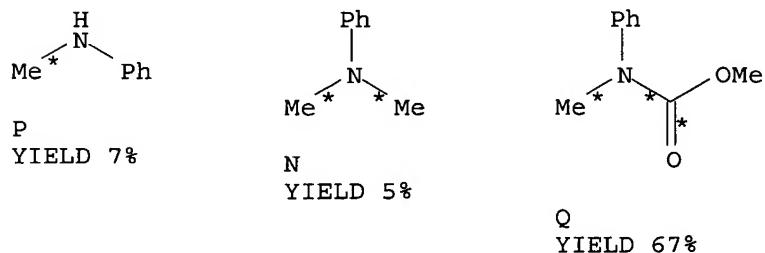
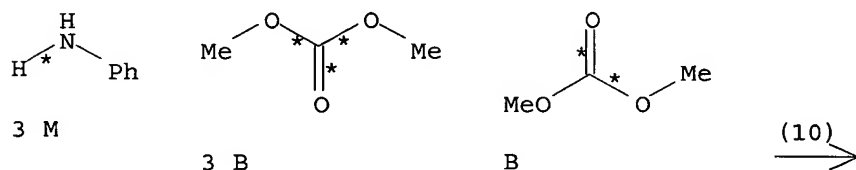
NTE stereoselective

ACCESSION NUMBER: 112:178775 CASREACT
 TITLE: Reactions with dimethyl carbonate. Part 3.
 Applications and mechanism of mono- or dimethylation
 of aromatic amines with dimethyl carbonate
 AUTHOR(S): Lissel, Manfred; Rohani-Dezfuli, Ali Reza; Vogt,
 Gabriele
 CORPORATE SOURCE: Fak. Chem., Univ. Bielefeld, Bielefeld, D-4800/1, Fed.
 Rep. Ger.
 SOURCE: Journal of Chemical Research, Synopses (1989), (10),
 312
 CODEN: JRPSDC; ISSN: 0308-2342
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



AB Methylation of aminoantipyrine I ($R = R_1 = H$) with di-Me carbonate (II) in the presence of K_2CO_3 and 18-crown-6 at 90° , gave I ($R = Me, R_1 = CO_2Me$), which on hydrolysis with 10% KOH gave I ($R = Me, R_1 = H$). At 50° , I ($R = R_1 = H$) reacted with II in the presence of NaH, and 18-crown-6 to give I ($R = H, R_1 = CO_2Me$). Other aromatic amines, e.g., 4- $R_2C_6H_4NH_2$ ($R_2 = H, Me, Cl$), were also N-methylated with II. The mechanism of the reactions is discussed.

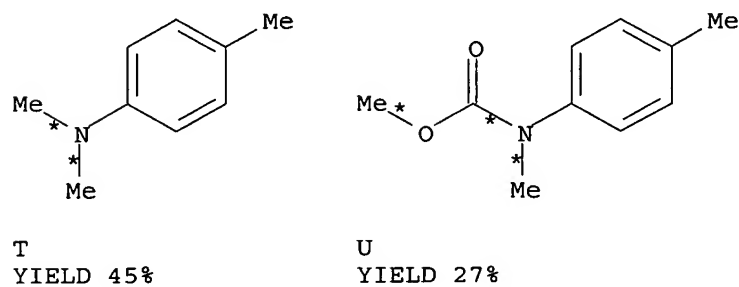
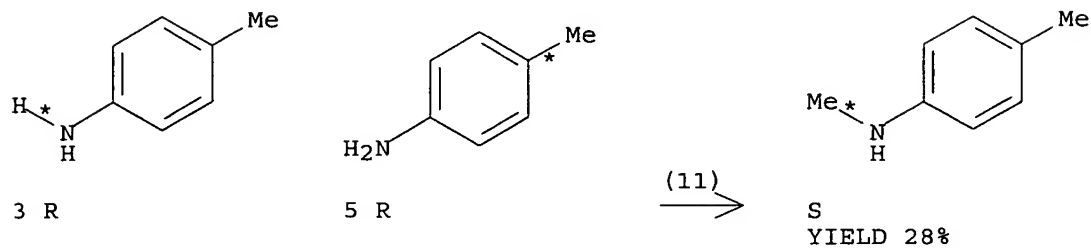
RX(10) OF 21 3 M + 4 B ==> P + N + Q



RX(10) RCT M 62-53-3, B 616-38-6
 RGT D 584-08-7 K_2CO_3

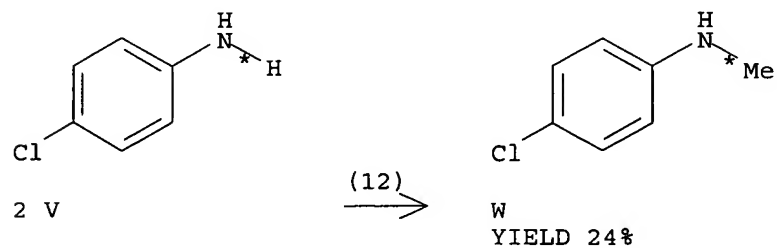
PRO P 100-61-8, N 121-69-7, Q 28685-60-1
 CAT 17455-13-9 18-Crown-6
 SOL 616-38-6 Me₂CO₃
 NTE product varies with reaction conditions

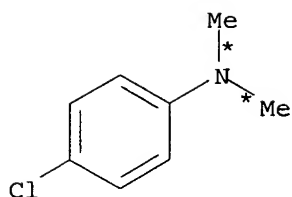
RX(11) OF 21 8 R ==> S + T + U



RX(11) RCT R 106-49-0
 RGT B 616-38-6 Me₂CO₃
 PRO S 623-08-5, T 99-97-8, U 121825-89-6
 SOL 616-38-6 Me₂CO₃

RX(12) OF 21 2 V ==> W + X





X
YIELD 12%

RX(12) RCT V 106-47-8
RGT B 616-38-6 Me2CO3
PRO W 932-96-7, X 698-69-1
SOL 616-38-6 Me2CO3

L60 ANSWER 38 OF 44 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 110:75136 CASREACT

TITLE: Selective protection of polyamines: Synthesis of model compounds and spermidine derivatives

AUTHOR(S): Almeida, M. Lurdes S.; Grehn, Leif; Ragnarsson, Ulf

CORPORATE SOURCE: Biomed. Cent., Univ. Uppsala, Uppsala, S-751 23, Swed.

SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1988), (7), 1905-11

CODEN: JCPRB4; ISSN: 0300-922X

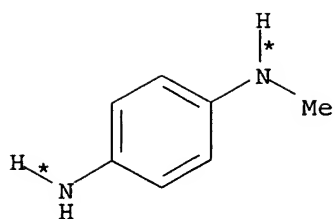
DOCUMENT TYPE: Journal

LANGUAGE: English

AB A general procedure for the selective protection of mixed primary-secondary (poly)amines, based on tert-butoxycarbonylation of carbamate groups (exhaustive tert-butoxycarbonylation) derived from the primary amino functions only, is reported. In most cases, benzyl (poly)carbamates are used for this purpose. Subsequent removal of all benzyloxycarbonyl (Z) groups from the resulting intermediates by catalytic hydrogenolysis liberates the secondary amino functions, while tert-butoxycarbonyl (Boc) is retained on the primary ones. Alternatively, selective removal of Z only from amino functions protected by both Z and Boc, which can be accomplished by base-catalyzed methanolysis, results in protected (poly)amines with Boc and Z on their primary and secondary amino groups, resp. The new reactions have been studied with two unsym. derivs. of ethylenediamine and p-phenylenediamine as model substances. The yields of most intermediates and the products were high. Addnl. expts. performed with spermidine gave N1,N8-Boc2-spermidine. The synthesis of N8-Boc-N1-Z-spermidine by the same approach is presented.

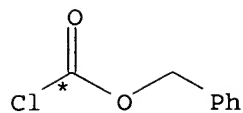
RX(60) OF 65 COMPOSED OF RX(18), RX(19), RX(20)

RX(60) AL + 2 B + H ==> AO

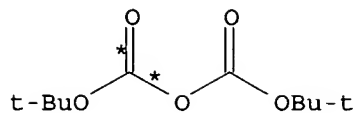


● HCl

AL

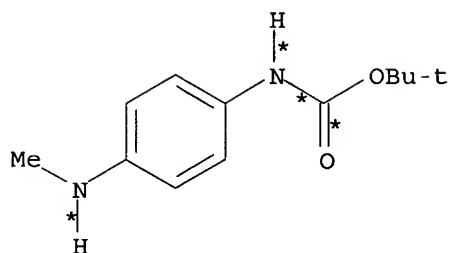


2 B



H

3
STEPS
→



AO
YIELD 98%

RX(18) RCT AL 118734-05-7, B 501-53-1
RGT AF 110-86-1 Pyridine
PRO AM 113283-90-2
SOL 110-86-1 Pyridine

RX(19) RCT AM 113283-90-2, H 24424-99-5
RGT J 1122-58-3 4-DMAP
PRO AN 113283-92-4
SOL 75-05-8 MeCN

RX(20) RCT AN 113283-92-4
RGT AP 1333-74-0 H2
PRO AO 113283-94-6
CAT 7440-05-3 Pd
SOL 67-56-1 MeOH

L60 ANSWER 39 OF 44 CASREACT COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 110:172770 CASREACT
TITLE: Selective monoalkylation of amines
AUTHOR(S): Dalla Croce, Piero; La Rosa, Concetta; Ritieni,

Alberto
 CORPORATE SOURCE: Dip. Chim. Org. Ind., Cent. CNR, Milan, 20133, Italy
 SOURCE: Journal of Chemical Research, Synopses (1988), (10),
 346-7

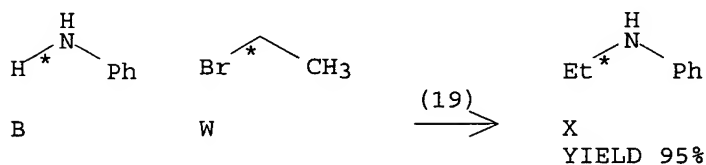
CODEN: JRPSDC; ISSN: 0308-2342

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A simple method for the monoalkylation of primary amines is achieved by using N-tert-butoxycarbonyl (N-Boc) group as a protecting group. The reaction of RNH₂ (R = Ph, substituted Ph, PhCH₂, cyclohexyl, Bu) with di-tert-Bu dicarbonate gave the N-Boc derivative in almost quant. yield. Treatment to the N-Boc derivs. with NaH, followed by alkyl halide and then hydrolysis of the product with 10% aqueous HCl gave RNHR₁ (R₁ = Et, Me, Pr, Bu, PhCH₂, allyl).

RX(19) OF 40 B + W ==> X



RX(19) RCT B 62-53-3

STAGE(1)

RGT A 24424-99-5 (Boc) 20

SOL 109-99-9 THF

STAGE(2)

RGT Y 7646-69-7 NaH

STAGE(3)

RCT W 74-96-4

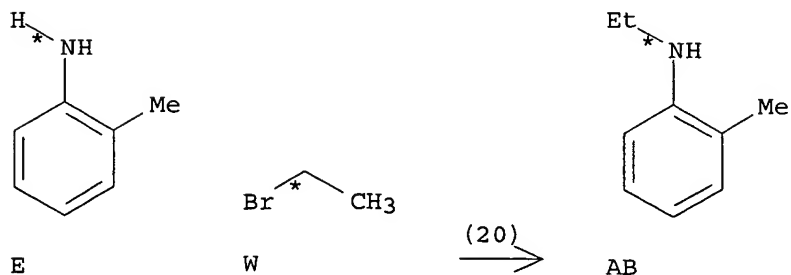
STAGE(4)

RGT Z 7647-01-0 HCl

SOL 7732-18-5 Water

PRO X 103-69-5

RX(20) OF 40 E + W ==> AB



RX(20) RCT E 95-53-4

STAGE(1)

RGT A 24424-99-5 (Boc)2O

SOL 109-99-9 THF

STAGE(2)

RGT Y 7646-69-7 NaH

STAGE(3)

RCT W 74-96-4

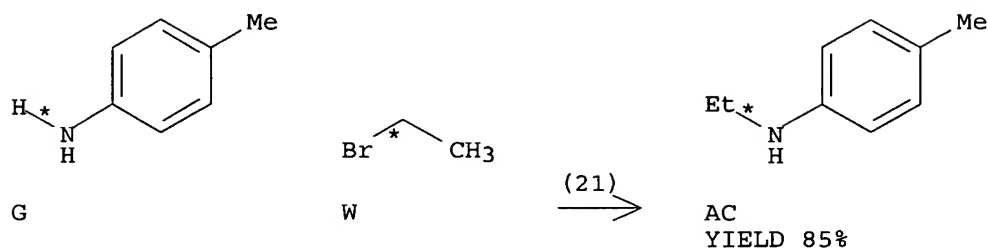
STAGE(4)

RGT Z 7647-01-0 HCl

SOL 7732-18-5 Water

PRO AB 94-68-8

RX(21) OF 40 G + W ==> AC



RX(21) RCT G 106-49-0

STAGE(1)

RGT A 24424-99-5 (Boc)2O

SOL 109-99-9 THF

STAGE(2)

RGT Y 7646-69-7 NaH

STAGE(3)

RCT W 74-96-4

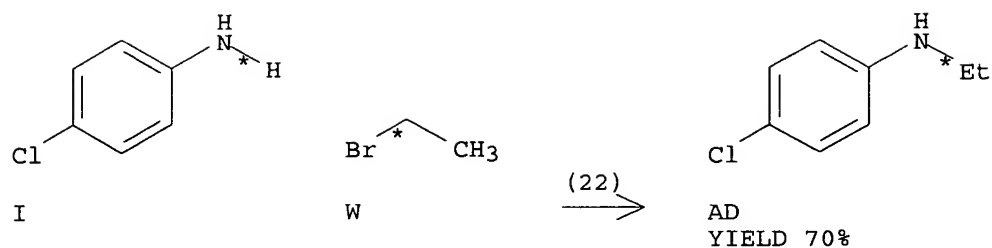
STAGE(4)

RGT Z 7647-01-0 HCl

SOL 7732-18-5 Water

PRO AC 622-57-1

RX(22) OF 40 I + W ==> AD



RX(22) RCT I 106-47-8

STAGE(1)

RGT A 24424-99-5 (Boc) 20

SOL 109-99-9 THF

STAGE(2)

RGT Y 7646-69-7 NaH

STAGE(3)

RCT W 74-96-4

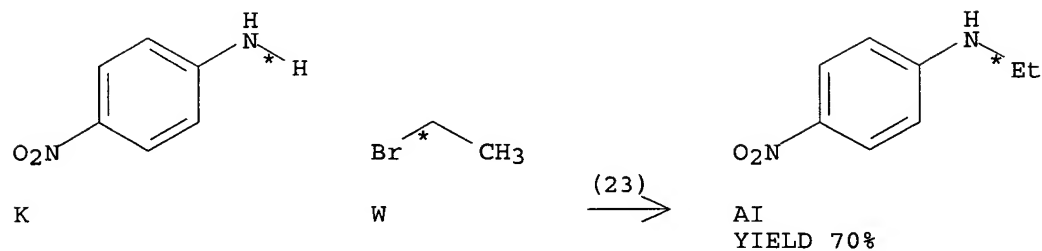
STAGE(4)

RGT Z 7647-01-0 HCl

SOL 7732-18-5 Water

PRO AD 13519-75-0

RX(23) OF 40 K + W ==> AI



RX(23) RCT K 100-01-6

STAGE(1)

RGT A 24424-99-5 (Boc) 20

SOL 109-99-9 THF

STAGE(2)

RGT Y 7646-69-7 NaH

STAGE(3)

RCT W 74-96-4

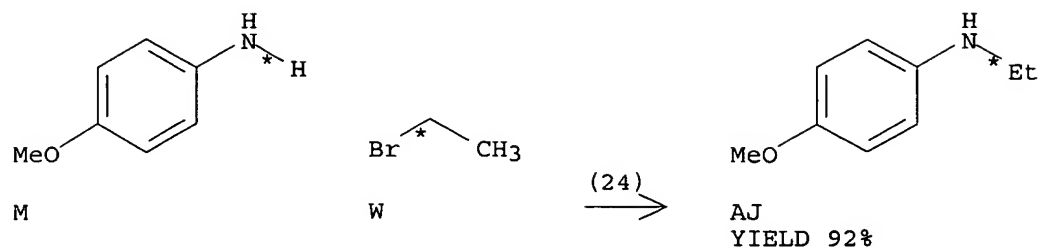
STAGE(4)

RGT Z 7647-01-0 HCl

SOL 7732-18-5 Water

PRO AI 3665-80-3

RX(24) OF 40 M + W ==> AJ



RX(24) RCT M 104-94-9

STAGE(1)

RGT A 24424-99-5 (Boc) 20

SOL 109-99-9 THF

STAGE(2)

RGT Y 7646-69-7 NaH

STAGE(3)

RCT W 74-96-4

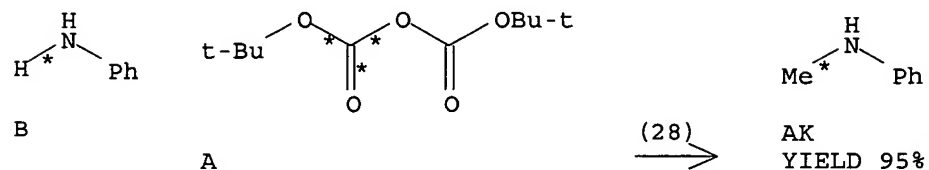
STAGE(4)

RGT Z 7647-01-0 HCl

SOL 7732-18-5 Water

PRO AJ 104-48-3

RX(28) OF 40 B + A ==> AK



RX(28) RCT B 62-53-3, A 24424-99-5

STAGE(1)

SOL 109-99-9 THF

STAGE(2)

RGT Y 7646-69-7 NaH

STAGE(3)

RGT AL 74-88-4 MeI

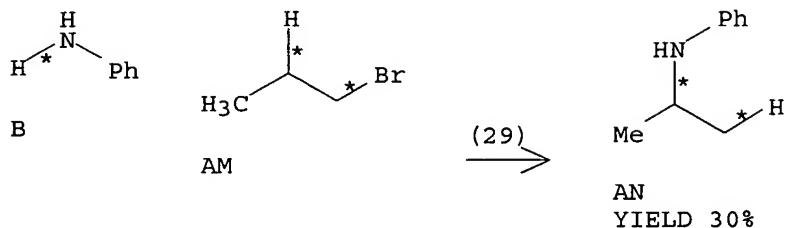
STAGE(4)

RGT Z 7647-01-0 HCl

SOL 7732-18-5 Water

PRO AK 100-61-8

RX(29) OF 40 B + AM ==> AN



RX(29) RCT B 62-53-3

STAGE(1)

RGT A 24424-99-5 (Boc) 20

SOL 109-99-9 THF

STAGE(2)

RGT Y 7646-69-7 NaH

STAGE(3)

RCT AM 106-94-5

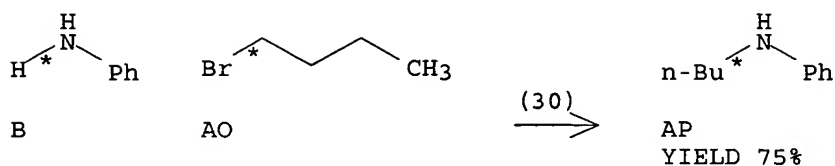
STAGE(4)

RGT Z 7647-01-0 HCl

SOL 7732-18-5 Water

PRO AN 768-52-5

RX(30) OF 40 B + AO ==> AP



RX(30) RCT B 62-53-3

STAGE(1)

RGT A 24424-99-5 (Boc) 20

SOL 109-99-9 THF

STAGE(2)

RGT Y 7646-69-7 NaH

STAGE(3)

RCT AO 109-65-9

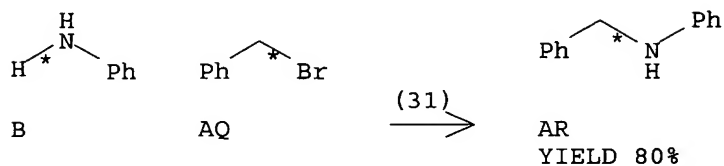
STAGE(4)

RGT Z 7647-01-0 HCl

SOL 7732-18-5 Water

PRO AP 1126-78-9

RX(31) OF 40 B + AQ ==> AR



RX(31) RCT B 62-53-3

STAGE(1)

RGT A 24424-99-5 (Boc)2O

SOL 109-99-9 THF

STAGE(2)

RGT Y 7646-69-7 NaH

STAGE(3)

RCT AQ 100-39-0

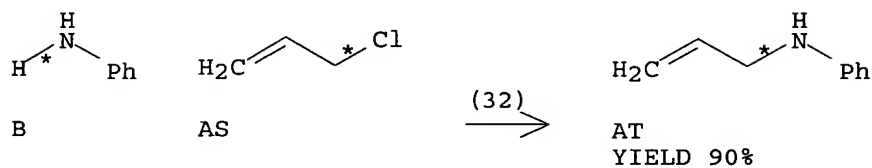
STAGE(4)

RGT Z 7647-01-0 HCl

SOL 7732-18-5 Water

PRO AR 103-32-2

RX(32) OF 40 B + AS ==> AT



RX(32) RCT B 62-53-3

STAGE(1)

RGT A 24424-99-5 (Boc)2O

SOL 109-99-9 THF

STAGE(2)

RGT Y 7646-69-7 NaH

STAGE(3)

RCT AS 107-05-1

STAGE(4)

RGT Z 7647-01-0 HCl

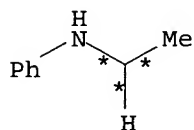
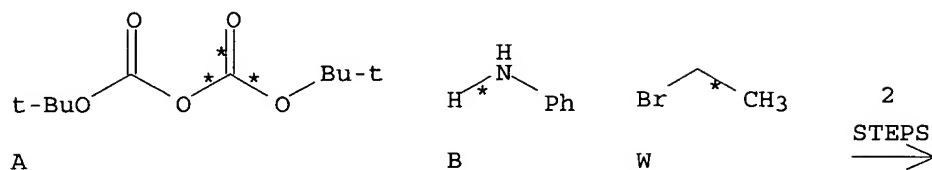
SOL 7732-18-5 Water

PRO AT 589-09-3

NTE Chloride assumed

RX(33) OF 40 COMPOSED OF RX(1), RX(11)

RX(33) A + B + W ==> X

X
YIELD 98%

RX(1) RCT A 24424-99-5, B 62-53-3
 PRO C 3422-01-3
 SOL 109-99-9 THF

RX(11) RCT C 3422-01-3

STAGE(1)

RGT Y 7646-69-7 NaH

SOL 109-99-9 THF

STAGE(2)

RCT W 74-96-4

RGT Z 7647-01-0 HCl

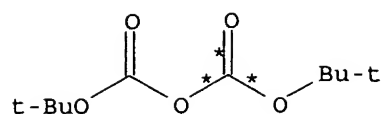
SOL 7732-18-5 Water

PRO X 103-69-5

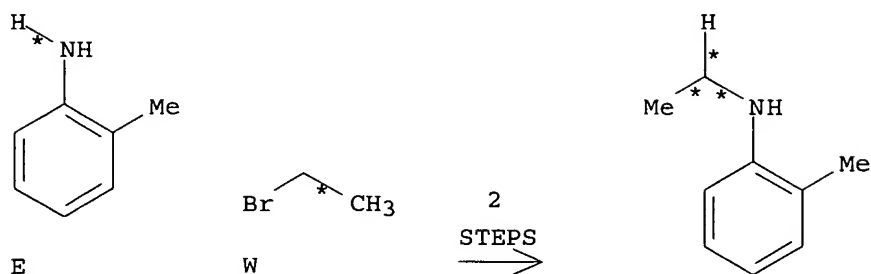
NTE Dioxane may also be used as solvent

RX(34) OF 40 COMPOSED OF RX(2), RX(12)

RX(34) A + E + W ==> AB



A

AB
YIELD 82%

RX(2) RCT A 24424-99-5, E 95-53-4
 PRO F 74965-31-4
 SOL 109-99-9 THF

RX(12) RCT F 74965-31-4

STAGE(1)

RGT Y 7646-69-7 NaH
 SOL 109-99-9 THF

STAGE(2)

RCT W 74-96-4

STAGE(3)

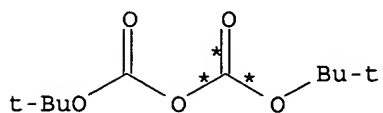
RGT Z 7647-01-0 HCl
 SOL 7732-18-5 Water

PRO AB 94-68-8

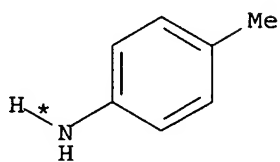
NTE Dioxane may also be used as solvent

RX(35) OF 40 COMPOSED OF RX(3), RX(13)

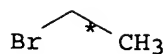
RX(35) A + G + W ==> AC



A

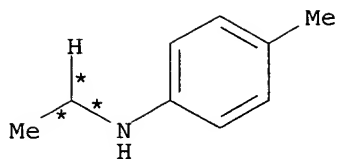


G



W

2
STEPS
→



AC
YIELD 91%

RX(3) RCT A 24424-99-5, G 106-49-0
PRO H 14618-59-8
SOL 109-99-9 THF

RX(13) RCT H 14618-59-8

STAGE(1)

RGT Y 7646-69-7 NaH
SOL 109-99-9 THF

STAGE(2)

RCT W 74-96-4

STAGE(3)

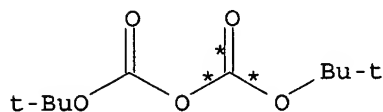
RGT Z 7647-01-0 HCl
SOL 7732-18-5 Water

PRO AC 622-57-1

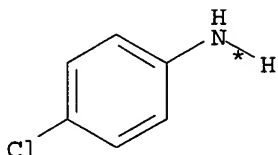
NTE Dioxane may also be used as solvent

RX(36) OF 40 COMPOSED OF RX(4), RX(14)

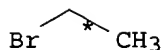
RX(36) A + I + W ==> AD



A

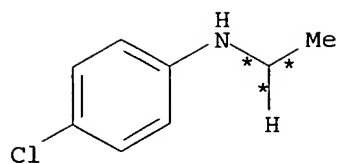


I



W

2
STEPS
→



AD
YIELD 73%

RX(4) RCT A 24424-99-5, I 106-47-8
PRO J 18437-66-6
SOL 109-99-9 THF

RX(14) RCT J 18437-66-6

STAGE(1)

RGT Y 7646-69-7 NaH
SOL 109-99-9 THF

STAGE(2)

RCT W 74-96-4

STAGE(3)

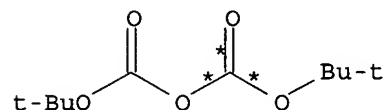
RGT Z 7647-01-0 HCl
SOL 7732-18-5 Water

PRO AD 13519-75-0

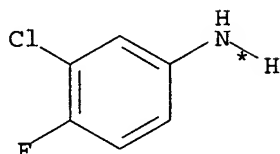
NTE Dioxane may also be used as solvent

RX(37) OF 40 COMPOSED OF RX(7), RX(15)

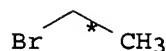
RX(37) A + O + W ==> AE



A

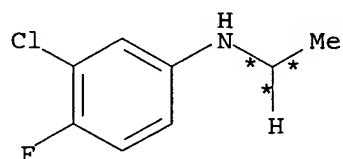


O



W

2
STEPS
→



AE
YIELD 87%

RX(7) RCT A 24424-99-5, O 367-21-5
 PRO P 119951-96-1
 SOL 109-99-9 THF

RX(15) RCT P 119951-96-1

STAGE(1)
 RGT Y 7646-69-7 NaH
 SOL 109-99-9 THF

STAGE(2)
 RCT W 74-96-4

STAGE(3)
 RGT Z 7647-01-0 HCl
 SOL 7732-18-5 Water

PRO AE 106847-36-3
 NTE Dioxane may also be used as solvent

L60 ANSWER 40 OF 44 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 108:112816 CASREACT

TITLE: Selective protection of mixed primary-secondary amines. Simple preparation of N1,N8-bis(tert-butyloxycarbonyl)spermidine

AUTHOR(S): Almeida, M. Lurdes S.; Grehn, Leif; Ragnarsson, Ulf
 CORPORATE SOURCE: Inst. Biochem., Univ. Uppsala, Uppsala, S-751 23, Swed.

SOURCE: Journal of the Chemical Society, Chemical Communications (1987), (16), 1250-1
 CODEN: JCCCAT; ISSN: 0022-4936

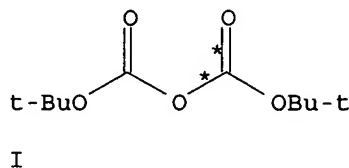
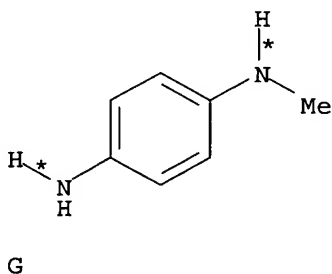
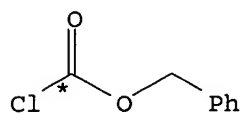
DOCUMENT TYPE: Journal

LANGUAGE: English

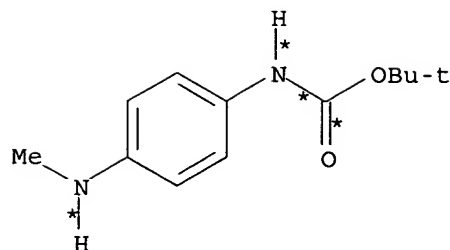
AB A procedure for the selective protection of mixed primary-secondary amines, based on acylation followed by exhaustive tert-butoxycarbonylation is presented. Thus, $\text{H}_2\text{N}(\text{CH}_2)_3\text{NH}(\text{CH}_2)_4\text{NH}_2$ was treated with $\text{PhCH}_2\text{O}_2\text{CCl}$ and aqueous Na_2CO_3 , followed by $(\text{Me}_3\text{CO})_2\text{CO}$ and 4-(dimethylamino)pyridine to give $\text{RR}_1\text{N}(\text{CH}_2)_3\text{NR}_2(\text{CH}_2)_4\text{NRR}_1$ (I, $\text{R} = \text{R}_2 = \text{PhCH}_2\text{O}_2\text{C}$, $\text{R}_1 = \text{Me}_3\text{CO}_2\text{C}$). Transfer hydrogenation of the latter compound using HCO_2NH_4 and Pd-C in MeOH gave I ($\text{R} = \text{R}_2 = \text{H}$, $\text{R}_1 = \text{Me}_3\text{CO}_2\text{C}$), whereas, treatment with $\text{Me}_2\text{NC}(:\text{NH})\text{NMe}_2$ in MeOH gave I ($\text{R} = \text{H}$, $\text{R}_1 = \text{Me}_3\text{CO}_2\text{C}$, $\text{R}_2 = \text{PhCH}_2\text{O}_2\text{C}$).

RX(29) OF 34 COMPOSED OF RX(3), RX(6), RX(8)

RX(29) 2 A + G + I ==> R



3
STEPS
→



R
YIELD 98%

RX(3) RCT A 501-53-1, G 623-09-6
RGT D 110-86-1 Pyridine
PRO H 113283-90-2

RX(6) RCT I 24424-99-5, H 113283-90-2
RGT K 1122-58-3 4-DMAP
PRO M 113283-92-4
SOL 75-05-8 MeCN

RX(8) RCT M 113283-92-4
RGT S 1333-74-0 H2
PRO R 113283-94-6
CAT 7440-05-3 Pd
SOL 67-56-1 MeOH

L60 ANSWER 41 OF 44 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 104:224725 CASREACT

TITLE: Carbamates

INVENTOR(S): Frulla, Floro F.; Stuber, Fred A.; Whitman, Peter J.

PATENT ASSIGNEE(S): Dow Chemical Co., USA

SOURCE: U.S., 5 pp.

CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

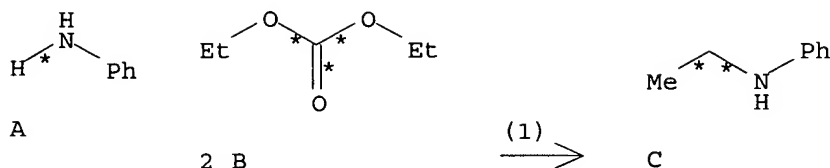
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4550188	A	19851029	US 1984-625060	19840627
PRIORITY APPLN. INFO.:			US 1984-625060	19840627

AB Carbamates useful as precursors for insecticides and as intermediates for organic mono- and polyisocyanates (no data) are manufactured at low temps. and in

high yields by heating an organic carbonate, i.e. a dialkyl, diaryl, diaralkyl, or cyclic carbonate ester, with an aromatic primary amine at 75-200° in the presence of Al metal catalyst with a promoter containing a Hg salt compound and iodine. Thus, a flask containing aniline 7.5, di-Et carbonate 96.2, Al foil 0.5, iodine 0.01, and HgCl₂ 0.01 g was heated at 130° for 17.5 h, diluted with 200 mL H₂O, and extracted to give 11.6 g residue containing 92.4% Et N-phenylcarbamate and 0.7% diphenylurea. Similarly, CH₂(C₆H₄NHCO₂Et)₂ was prepared in 85.8% yield.

RX(1) OF 2 A + 2 B ==> C



RX(1) RCT A 62-53-3, B 105-58-8
 PRO C 103-69-5

L60 ANSWER 42 OF 44 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2006:117009 CAPLUS

DOCUMENT NUMBER: 144:212531

TITLE: Catalytic method for the production of monoalkylated
 (hetero)aromatic diamines using **carbonates**
 and (hetero)aryl diamines

INVENTOR(S): Russ, Werner Hubert; Hutchings, Michael; Ebenezer,
 Warren James

PATENT ASSIGNEE(S): Dystar Textilfarben G.m.b.H. & Co. Deutschland K.-G.,
 Germany

SOURCE: PCT Int. Appl., 12 pp.
 CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006013164	A1	20060209	WO 2005-EP53591	20050722
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
DE 102004036787	A1	20060323	DE 2004-102004036787	20040729

PRIORITY APPLN. INFO.: DE 2004-102004036787A 20040729

OTHER SOURCE(S): MARPAT 144:212531

AB Monoalkylated aromatic diamines [e.g., 2-(methylanino)aniline] are prepared by the monoalkylation of a (hetero)aromatic diamine (e.g., o-phenylenediamine) with a cyclic or diorganyl **carbonate** (e.g., di-Me **carbonate**) in the presence of a zeolite catalyst (e.g., NaY-faujasite-type zeolite).

IC ICM C07C209-00

ICS C07C211-51

CC 25-4 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)

Section cross-reference(s): 45, 67

IT **Faujasite-type zeolites**
 RL: CAT (Catalyst use); USES (Uses)
 (NaY-**faujasite**; catalysts in a method for the production of monoalkylated (hetero)aromatic diamines using **carbonates** and (hetero)aryl diamines)

IT **Zeolites (synthetic), uses**
 RL: CAT (Catalyst use); USES (Uses)
 (catalysts in a method for the production of monoalkylated (hetero)aromatic diamines using **carbonates** and (hetero)aryl diamines)

IT **Carbonates, reactions**
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (catalytic method for the production of monoalkylated (hetero)aromatic diamines using **carbonates** and (hetero)aryl diamines)

IT **Amines, preparation**
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (diamines, **aromatic**, monoalkylated; catalytic method for the production of monoalkylated (hetero)**aromatic** diamines using **carbonates** and (hetero)aryl diamines)

IT **Alkylation**
 (monoalkylation; catalytic method for the production of monoalkylated (hetero)aromatic diamines using **carbonates** and (hetero)aryl diamines)

IT **Alkylation catalysts**
 (monoalkylation; zeolites in a method for the production of monoalkylated (hetero)aromatic diamines using **carbonates** and (hetero)aryl diamines)

IT 554-13-2, Lithium **carbonate** 5006-97-3, Lithium **bicarbonate**
 RL: CAT (Catalyst use); USES (Uses)
 (catalysts in a method for the production of monoalkylated (hetero)aromatic diamines using **carbonates** and (hetero)aryl diamines)

IT 95-54-5, o-Phenylenediamine, reactions 96-49-1, Ethylene **carbonate** 616-38-6, Dimethyl **carbonate**
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (catalytic method for the production of monoalkylated (hetero)aromatic diamines using **carbonates** and (hetero)aryl diamines)

IT 4760-34-3P, 2-(Methylamino)aniline
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (catalytic method for the production of monoalkylated (hetero)aromatic diamines using **carbonates** and (hetero)aryl diamines)

REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L60 ANSWER 43 OF 44 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1995:376454 CAPLUS

DOCUMENT NUMBER: 122:164029

TITLE: Selectivity to N-mono or dialkylation in the reaction of aniline with dimethyl **carbonate** on **faujasite**, EMT and beta alkaline zeolites

AUTHOR(S): Rao, P. R. Hari Prasad; Massiani, Pascale; Barthomeuf, Denise

CORPORATE SOURCE: Lab. Reactivite Surface, Univ. Pierre Marie Curie, Paris, 75252, Fr.

SOURCE: Catalysis Letters (1995), 31(1), 115-20

CODEN: CALEER; ISSN: 1011-372X

PUBLISHER: Baltzer

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Zeolite K-EMT is as active and selective to N-monomethylation as KY in the

alkylation of aniline with di-Me **carbonate** at 408 or 453 K. No C-alkylation occurs in the temperature range studied. At 503 K, KX and CsX are about 75% selective for dialkylation to N,N-dimethylaniline with about 97% conversion.

CC 45-4 (Industrial Organic Chemicals, Leather, Fats, and Waxes)

Section cross-reference(s): 67

IT Zeolites, uses

RL: CAT (Catalyst use); USES (Uses)

(Cs EMT-type; selectivity to N-mono- or dialkylation of aniline with di-Me **carbonate** over **faujasite**, EMT, and beta alkaline zeolites)

IT Zeolites, uses

RL: CAT (Catalyst use); USES (Uses)

(Cs beta; selectivity to N-mono- or dialkylation of aniline with di-Me **carbonate** over **faujasite**, EMT, and beta alkaline zeolites)

IT Zeolites, uses

RL: CAT (Catalyst use); USES (Uses)

(K EMT-type; selectivity to N-mono- or dialkylation of aniline with di-Me **carbonate** over **faujasite**, EMT, and beta alkaline zeolites)

IT Alkylation

Alkylation catalysts

(selectivity to N-mono- or dialkylation of aniline with di-Me **carbonate** over **faujasite**, EMT, and beta alkaline zeolites)

IT Zeolites, uses

RL: CAT (Catalyst use); USES (Uses)

(CsX, selectivity to N-mono- or dialkylation of aniline with di-Me **carbonate** over **faujasite**, EMT, and beta alkaline zeolites)

IT Zeolites, uses

RL: CAT (Catalyst use); USES (Uses)

(CsY, selectivity to N-mono- or dialkylation of aniline with di-Me **carbonate** over **faujasite**, EMT, and beta alkaline zeolites)

IT Zeolites, uses

RL: CAT (Catalyst use); USES (Uses)

(H beta, selectivity to N-mono- or dialkylation of aniline with di-Me **carbonate** over **faujasite**, EMT, and beta alkaline zeolites)

IT Zeolites, uses

RL: CAT (Catalyst use); USES (Uses)

(K beta, selectivity to N-mono- or dialkylation of aniline with di-Me **carbonate** over **faujasite**, EMT, and beta alkaline zeolites)

IT Zeolites, uses

RL: CAT (Catalyst use); USES (Uses)

(KX, selectivity to N-mono- or dialkylation of aniline with di-Me **carbonate** over **faujasite**, EMT, and beta alkaline zeolites)

IT Zeolites, uses

RL: CAT (Catalyst use); USES (Uses)

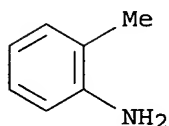
(KY, selectivity to N-mono- or dialkylation of aniline with di-Me **carbonate** over **faujasite**, EMT, and beta alkaline zeolites)

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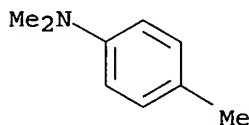
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(Na EMT-type, selectivity to N-mono- or dialkylation of aniline with di-Me **carbonate** over **faujasite**, EMT, and beta alkaline zeolites)

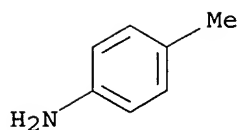
- zeolites)
- IT Zeolites, uses
 RL: CAT (Catalyst use); USES (Uses)
 (Na beta, selectivity to N-mono- or dialkylation of aniline with di-Me carbonate over faujasite, EMT, and beta alkaline zeolites)
- IT 95-53-4P, o-Toluidine, preparation 99-97-8P,
 N,N-Dimethyl-p-toluidine 106-49-0P, p-Toluidine, preparation
 RL: BYP (Byproduct); PREP (Preparation)
 (selectivity to N-mono- or dialkylation of aniline with di-Me carbonate over faujasite, EMT, and beta alkaline zeolites)
- IT 100-61-8P, N-Methylaniline, preparation 121-69-7P,
 N,N-Dimethylaniline, preparation
 RL: IMF (Industrial manufacture); PREP (Preparation)
 (selectivity to N-mono- or dialkylation of aniline with di-Me carbonate over faujasite, EMT, and beta alkaline zeolites)
- IT 62-53-3, Aniline, reactions 616-38-6, Dimethyl carbonate
 RL: PEP (Physical, engineering or chemical process); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
 (selectivity to N-mono- or dialkylation of aniline with di-Me carbonate over faujasite, EMT, and beta alkaline zeolites)
- IT 95-53-4P, o-Toluidine, preparation 99-97-8P,
 N,N-Dimethyl-p-toluidine 106-49-0P, p-Toluidine, preparation
 RL: BYP (Byproduct); PREP (Preparation)
 (selectivity to N-mono- or dialkylation of aniline with di-Me carbonate over faujasite, EMT, and beta alkaline zeolites)
- RN 95-53-4 CAPLUS
 CN Benzenamine, 2-methyl- (9CI) (CA INDEX NAME)



- RN 99-97-8 CAPLUS
 CN Benzenamine, N,N,4-trimethyl- (9CI) (CA INDEX NAME)



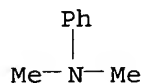
- RN 106-49-0 CAPLUS
 CN Benzenamine, 4-methyl- (9CI) (CA INDEX NAME)



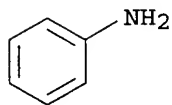
IT 100-61-8P, N-Methylaniline, preparation 121-69-7P,
 N,N-Dimethylaniline, preparation
 RL: IMF (Industrial manufacture); **PREP (Preparation)**
 (selectivity to N-mono- or dialkylation of aniline with di-Me
carbonate over **faujasite**, EMT, and beta alkaline
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 CN Benzenamine, N-methyl- (9CI) (CA INDEX NAME)

Me-NH-Ph

RN 121-69-7 CAPLUS
 CN Benzenamine, N,N-dimethyl- (9CI) (CA INDEX NAME)



IT 62-53-3, Aniline, reactions
 RL: PEP (Physical, engineering or chemical process); **RCT**
(Reactant); PROC (Process); **RACT (Reactant or reagent)**
 (selectivity to N-mono- or dialkylation of aniline with di-Me
carbonate over **faujasite**, EMT, and beta alkaline
 zeolites)
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 CN Benzenamine (9CI) (CA INDEX NAME)

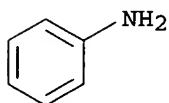


L60 ANSWER 44 OF 44 CAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 1993:519064 CAPLUS
 DOCUMENT NUMBER: 119:119064
 TITLE: Process for reclaiming a thermoset polymer
 INVENTOR(S): Jones, C. Andrew; Gaffney, Anne M.; Leyshon, David W.;
 Cozzone, Glenn E.; Sofranko, John A.
 PATENT ASSIGNEE(S): ACRO Chemical Technology, L. P., USA
 SOURCE: U.S., 10 pp.
 CODEN: USXXAM
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

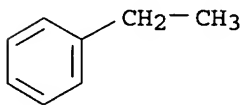
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5192809	A	19930309	US 1992-860638	19920330
PRIORITY APPLN. INFO.:			US 1992-860638	19920330

AB Filled thermosetting polymer waste is reclaimed by contacting polymer and particulate zeolite-containing catalyst in a fluidized bed at a temperature to give a coarse filler, coke, a volatile organic matter and a spent catalyst. The first stream comprising the volatile organic matter is withdrawn from the reaction zone, and then a second stream containing the other components; the second stream is heated in presence of O₂ to convert coke to CO₂ and H₂O and to regenerate catalyst, which is separated along with filler. Thus, volatile orgs. were recovered by heating glass fiber-filled maleic anhydride-styrene copolymer at 21-681° in presence of zeolite-containing catalyst; mass balance was 96% and O₂ balance was 100%.

IC ICM C08L101-00
INCL 521040000
CC 38-3 (Plastics Fabrication and Uses)
IT 12173-28-3, Faujasite 12173-98-7, Mordenite 12417-81-1, Offretite 12510-42-8, Erionite
RL: CAT (Catalyst use); USES (Uses)
(catalysts, for reclamation of volatile orgs. from thermosets)
IT 62-53-3P, Aniline, uses 100-41-4P, Ethylbenzene, uses
RL: PREP (Preparation); USES (Uses)
(reclamation recovery of, from thermosets, using zeolite catalysts)
IT 471-34-1, Calcium carbonate, uses
RL: USES (Uses)
(thermosets filled by, reclamation of, using zeolite catalysts)
IT 62-53-3P, Aniline, uses 100-41-4P, Ethylbenzene, uses
RL: PREP (Preparation); USES (Uses)
(reclamation recovery of, from thermosets, using zeolite catalysts)
RN 62-53-3 CAPLUS
CN Benzenamine (9CI) (CA INDEX NAME)



RN 100-41-4 CAPLUS
CN Benzene, ethyl- (7CI, 8CI, 9CI) (CA INDEX NAME)



AUTHOR SEARCH

Shiao 10/734208

05/03/2006

=> file casreact

FILE 'CASREACT' ENTERED AT 16:00:03 ON 03 MAY 2006

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FILE CONTENT:1840 - 30 Apr 2006 VOL 144 ISS 18

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*
*      CASREACT now has more than 10 million reactions      *
*
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Some CASREACT records are derived from the ZIC/VINITI database (1974-1991) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d stat que L39

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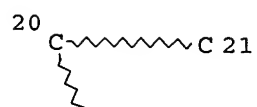
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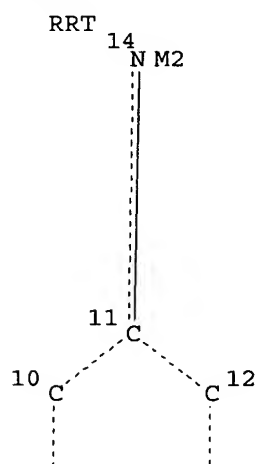
27 C M1

Page 1-A

23 C \equiv G1 24



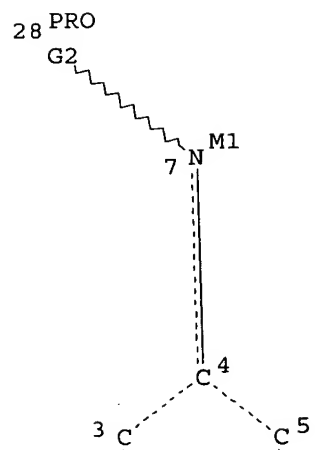
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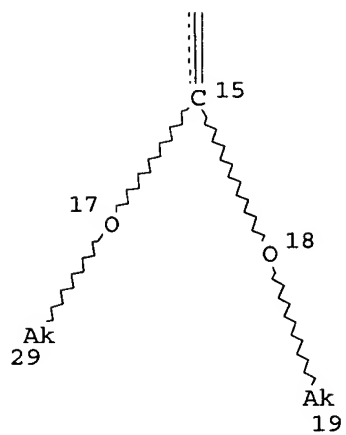
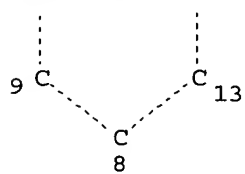
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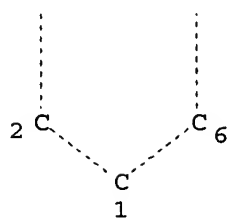
Page 2-A



Page 2-B



Page 3-A



Page 3-B

VAR G1=30/31

VAR G2=20/23/25/26/27

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NUMBER OF NODES IS 31

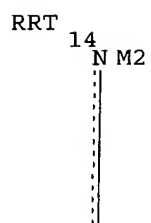
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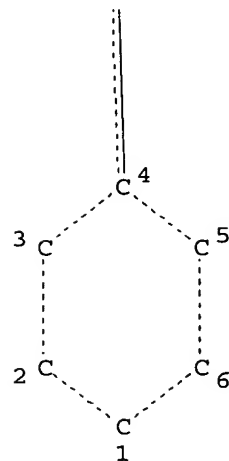
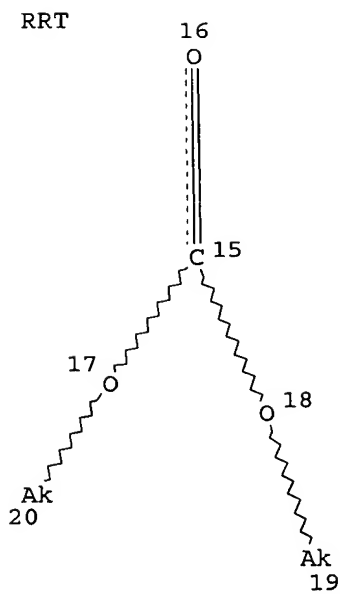
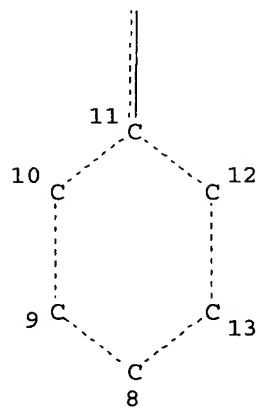
L34 STR

Ak 21

22 Ak~~~~~Cb 23



Page 1-A



Page 2-A
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DEFAULT ECLEVEL IS LIMITED
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GRAPH ATTRIBUTES:

RSPEC I

NUMBER OF NODES IS 24

STEREO ATTRIBUTES: NONE

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L38 57 SEA FILE=CASREACT ABB=ON PLU=ON TUNDO P?/AU
L39 7 SEA FILE=CASREACT ABB=ON PLU=ON L36 AND (L37 OR L38)
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=> file caplus

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FILE COVERS 1907 - 3 May 2006 VOL 144 ISS 19
FILE LAST UPDATED: 2 May 2006 (20060502/ED)

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L11     23 SEA FILE=CAPLUS ABB=ON PLU=ON L8 AND L10
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 L51 86 SEA FILE=CAPLUS ABB=ON PLU=ON L18 AND L8
 L52 6 SEA FILE=CAPLUS ABB=ON PLU=ON L51 AND L10
 L53 9721 SEA FILE=CAPLUS ABB=ON PLU=ON AMINES/CT (L) AROMATIC/OBI
 L54 5 SEA FILE=CAPLUS ABB=ON PLU=ON L51 AND L53
 L55 3 SEA FILE=CAPLUS ABB=ON PLU=ON L52 AND L54
 L56 8 SEA FILE=CAPLUS ABB=ON PLU=ON L19 OR L25 OR L26 OR L54 OR
 L55

L57 4 SEA FILE=CAPLUS ABB=ON PLU=ON (L40 OR L41) AND L56

=> dup rem L39 L57

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 PROCESSING COMPLETED FOR L39
 PROCESSING COMPLETED FOR L57

L61 9 DUP REM L39 L57 (2 DUPLICATES REMOVED)
ANSWERS '1-7' FROM FILE CASREACT
ANSWERS '8-9' FROM FILE CAPLUS

=> d ibib abs hit L61 1-7; d ibib abs hitind hitstr L61 8-9

L61 ANSWER 1 OF 9 CASREACT COPYRIGHT 2006 ACS on STN DUPLICATE 1
 ACCESSION NUMBER: 141:54061 CASREACT
 TITLE: Process and catalysts for the synthesis of
 mono-N-substituted functionalized anilines from
 anilines and carbonate esters

INVENTOR(S): Selva, Maurizio; Tundo, Pietro
PATENT ASSIGNEE(S): Consorzio Interuniversitario Nazionale la Chimica per
L'ambiente, Italy
SOURCE: Eur. Pat. Appl., 13 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

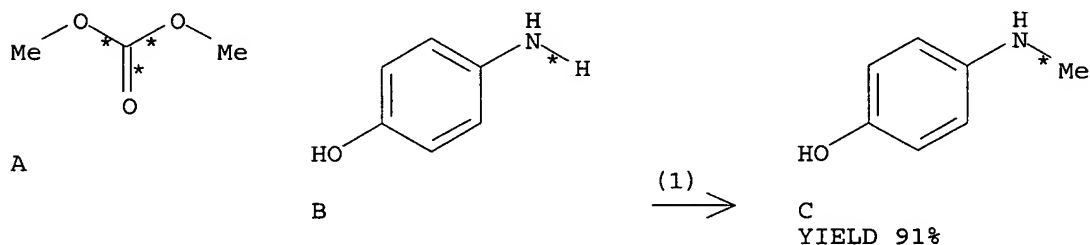
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1431274	A1	20040623	EP 2003-29005	20031216
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
US 2004127747	A1	20040701	US 2003- 734208	20031215
PRIORITY APPLN. INFO.:			IT 2002-PD325	20021218

OTHER SOURCE(S) : MARPAT 141:54061

AB A process for direct and selective synthesis of mono-N-substituted functionalized anilines [e.g., 4-(methylamino)phenol] comprises the alkylation of anilines (e.g., 4-hydroxyaniline) with organic carbonates in the presence of faujasite-type zeolite catalysts that are chemical exchanged with alkali metals (e.g., sodium).

REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX (1) OF 12 **A** + **B** ==> **C**

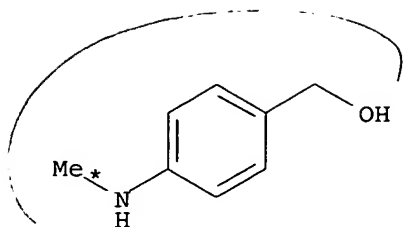


```

RX(1)      RCT  A 616-38-6, B 123-30-8
           PRO  C 150-75-4
           CAT  7440-23-5D Na
           SOL  110-71-4 (CH2OMe)2
           CON  SUBSTAGE(1) room temperature
              SUBSTAGE(2) room temperature -> 90 deg C
              SUBSTAGE(3) 7 hours
           NTE  NaY-faujasite was used as catalyst

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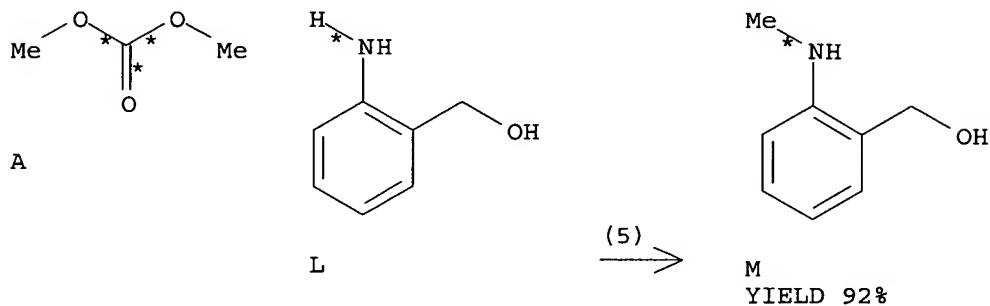
$$\text{RX (2) OF 12} \quad \mathbf{A} + \mathbf{F} ==> \mathbf{G}$$



K
YIELD 77%

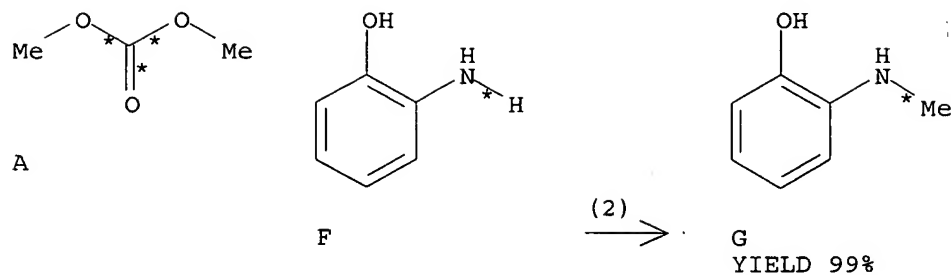
RX(4) RCT A 616-38-6, J 623-04-1
 PRO K 181819-75-0
 CAT 7440-23-5D Na
 SOL 616-38-6 Me2CO3
 CON SUBSTAGE(1) room temperature
 SUBSTAGE(2) room temperature -> 90 deg C
 SUBSTAGE(3) 8 hours
 NTE NaY-faujasite was used as catalyst

RX(5) OF 12 A + L ==> M



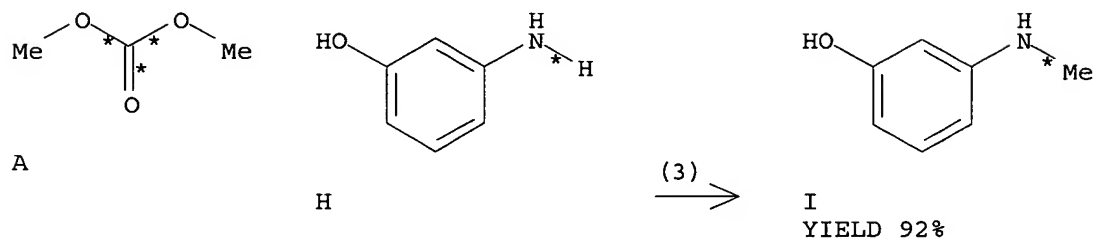
RX(5) RCT A 616-38-6, L 5344-90-1
 PRO M 29055-08-1
 CAT 7440-23-5D Na
 SOL 110-71-4 (CH2OMe)2
 CON SUBSTAGE(1) room temperature
 SUBSTAGE(2) room temperature -> 90 deg C
 SUBSTAGE(3) 7 hours
 NTE NaY-faujasite was used as catalyst

RX(6) OF 12 A + N ==> O



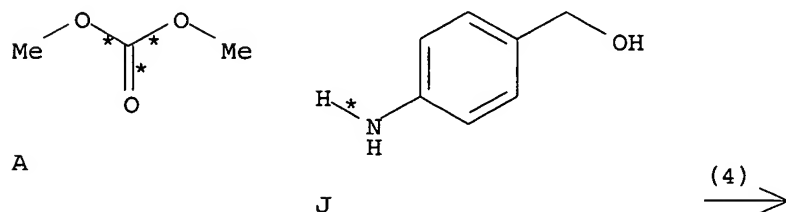
RX (2) RCT A 616-38-6, F 95-55-6
 PRO G 611-24-5
 CAT 7440-23-5D Na
 SOL 110-71-4 (CH₂OMe)₂
 CON SUBSTAGE(1) room temperature
 SUBSTAGE(2) room temperature -> 90 deg C
 SUBSTAGE(3) 3 hours
 NTE NaY-faujasite was used as catalyst

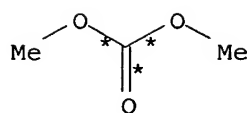
RX (3) OF 12 A + H ==> I



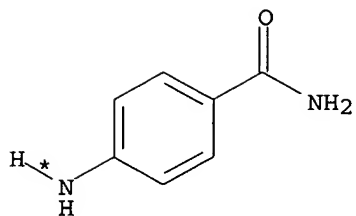
RX (3) RCT A 616-38-6, H 591-27-5
 PRO I 14703-69-6
 CAT 7440-23-5D Na
 SOL 616-38-6 Me₂CO₃
 CON SUBSTAGE(1) room temperature
 SUBSTAGE(2) room temperature -> 90 deg C
 SUBSTAGE(3) 7 hours
 NTE NaY-faujasite was used as catalyst

RX (4) OF 12 A + J ==> K

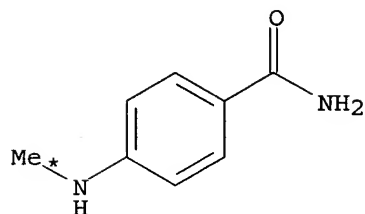




A



N

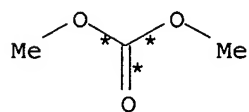
(6) \longrightarrow 

O

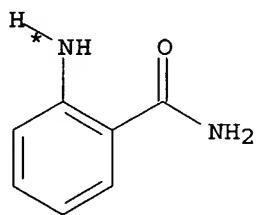
YIELD 86%

RX(6) RCT A 616-38-6, N 2835-68-9
 PRO O 38359-26-1
 CAT 7440-23-5D Na
 SOL 110-71-4 (CH₂OMe)₂
 CON SUBSTAGE(1) room temperature
 SUBSTAGE(2) room temperature -> 90 deg C
 SUBSTAGE(3) 7 hours
 NTE NaY-faujasite was used as catalyst

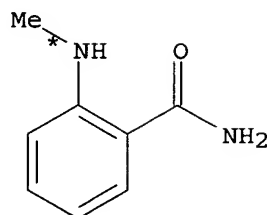
RX(7) OF 12 A + P ==> Q



A



P

(7) \longrightarrow 

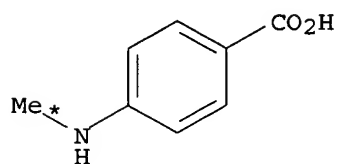
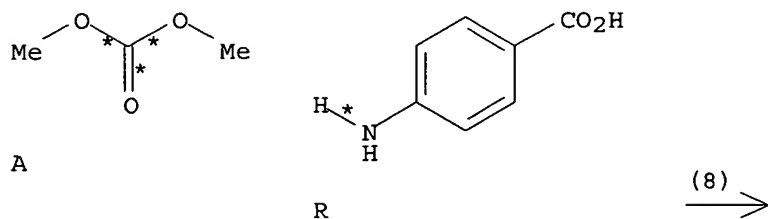
Q

YIELD 91%

RX(7) RCT A 616-38-6, P 88-68-6
 PRO Q 7505-81-9
 CAT 7440-23-5D Na
 SOL 110-71-4 (CH₂OMe)₂

CON SUBSTAGE(1) room temperature
 SUBSTAGE(2) room temperature -> 90 deg C
 SUBSTAGE(3) 22 hours
 NTE NaY-faujasite was used as catalyst

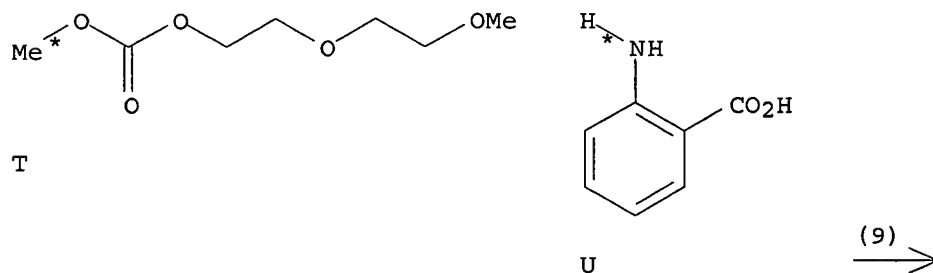
RX(8) OF 12 A + R ==> S

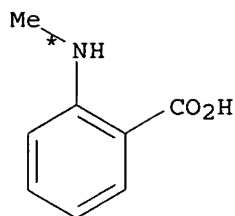


S
 YIELD 74%

RX(8) RCT A 616-38-6, R 150-13-0
 PRO S 10541-83-0
 CAT 7440-23-5D Na
 SOL 110-71-4 (CH₂OMe)₂
 CON SUBSTAGE(1) room temperature
 SUBSTAGE(2) room temperature -> 130 deg C
 SUBSTAGE(3) 9 hours
 NTE NaY-faujasite was used as catalyst

RX(9) OF 12 T + U ==> V

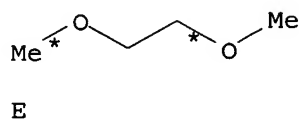
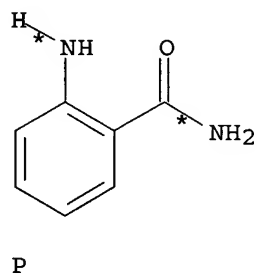
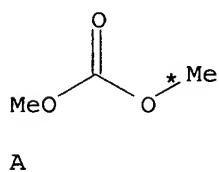




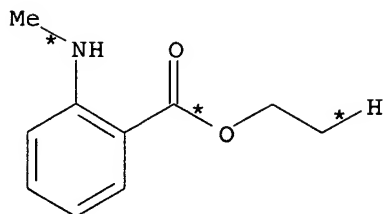
V
YIELD 93%

RX(9) RCT T 141814-27-9, U 118-92-3
 PRO V 119-68-6
 CAT 7440-23-5D Na
 SOL 112-49-2 Triglyme
 CON SUBSTAGE(1) room temperature
 SUBSTAGE(2) room temperature -> 150 deg C
 SUBSTAGE(3) 12 hours
 NTE NaY-faujasite was used as catalyst, thermal

RX(10) OF 12 A + P + E ==> X



(10) →

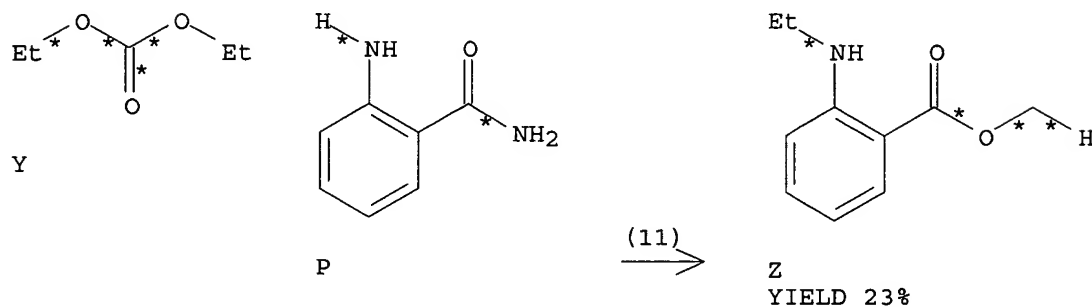


X
YIELD 65%

RX(10) RCT A 616-38-6, P 88-68-6, E 110-71-4
 PRO X 35472-56-1
 CAT 7440-23-5D Na
 SOL 110-71-4 (CH2OMe)2
 CON SUBSTAGE(1) room temperature

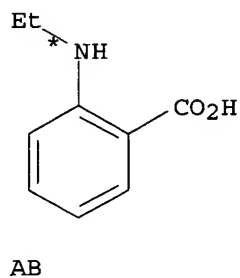
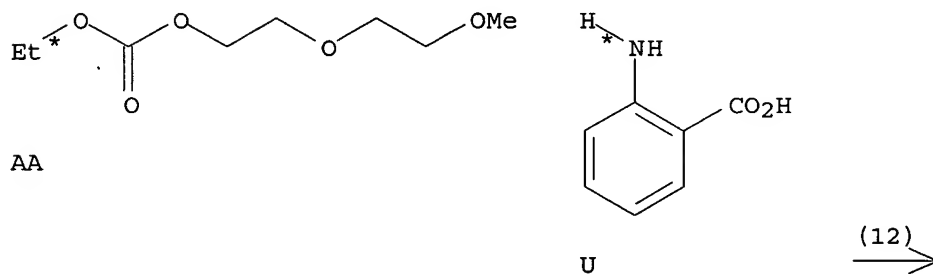
SUBSTAGE(2) room temperature -> 150 deg C
 SUBSTAGE(3) 8 hours
 NTE NaY-faujasite was used as catalyst, thermal

RX(11) OF 12 **Y + P ==> Z**



RX(11) RCT Y 105-58-8, P 88-68-6
 PRO Z 17318-49-9
 CAT 7440-23-5D Na
 SOL 110-71-4 (CH₂OMe)₂
 CON SUBSTAGE(1) room temperature
 SUBSTAGE(2) room temperature -> 150 deg C
 SUBSTAGE(3) 8 hours
 NTE NaY-faujasite was used as catalyst, thermal

RX(12) OF 12 **AA + U ==> AB**



RX(12) RCT AA 214470-03-8, U 118-92-3

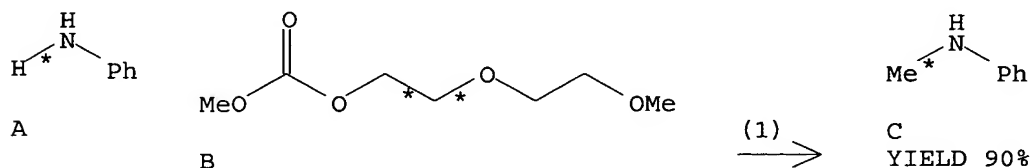
PRO AB 89-50-9
 CAT 7440-23-5D Na
 SOL 112-49-2 Triglyme
 CON SUBSTAGE(1) room temperature
 SUBSTAGE(2) room temperature -> 150 deg C
 SUBSTAGE(3) 18 hours
 NTE NaY-faujasite was used as catalyst, thermal
 IN Selva, Maurizio; Tundo, Pietro

L61 ANSWER 2 OF 9 CASREACT COPYRIGHT 2006 ACS on STN DUPLICATE 2
 ACCESSION NUMBER: 134:222468 CASREACT
 TITLE: Reaction of Primary Aromatic Amines with Alkyl
 Carbonates over NaY Faujasite: A Convenient and
 Selective Access to Mono-N-alkyl Anilines
 AUTHOR(S): Selva, Maurizio; Tundo, Pietro;
 Perosa, Alvisé
 CORPORATE SOURCE: Dipartimento di Scienze Ambientali, Università Ca'
 Foscari, Venice, 2137-30123, Italy
 SOURCE: Journal of Organic Chemistry (2001), 66(3), 677-680
 CODEN: JOCEAH; ISSN: 0022-3263
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB At atmospheric pressure and at 130-160 °C, primary aromatic amines (p-XC₆H₄NH₂, X = H, Cl, NO₂) are mono-N-alkylated in a single step, with sym. and asym. dialkyl carbonates [ROCOOR', R = Me, R' = MeO(CH₂)₂O(CH₂)₂; R = R' = Et; R = R' = benzyl; R = R' = allyl; R = Et, R' = MeO(CH₂)₂O(CH₂)₂], in the presence of a com. available NaY faujasite. No solvents are required. Mono-N-alkyl anilines are obtained with a very high selectivity (90-97%), in good to excellent yields (68-94%), on a preparative scale. In the presence of triglyme as a solvent, the mono-N-alkyl selectivity is independent of concentration and polarity factors. The reaction probably takes place within the polar zeolite cavities, and through the combined effect of the dual acid-base properties of the catalyst.

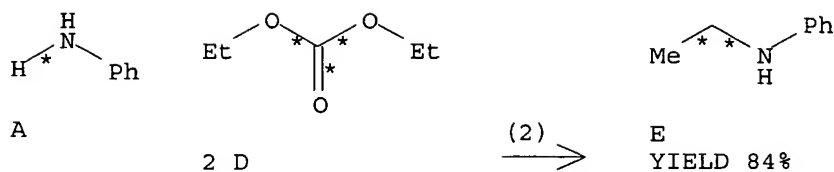
REFERENCE COUNT: 48 THERE ARE 48 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(1) OF 12 A + B ==> C



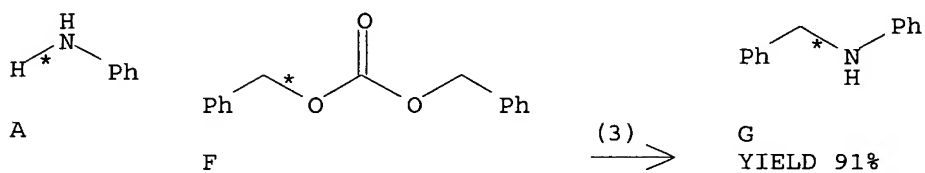
RX(1) RCT A 62-53-3, B 141814-27-9
 PRO C 100-61-8
 NTE NaY faujasite catalyst used; no solvent; thermal;
 regioselective; green chem.-waste redn.

RX(2) OF 12 A + 2 D ==> E



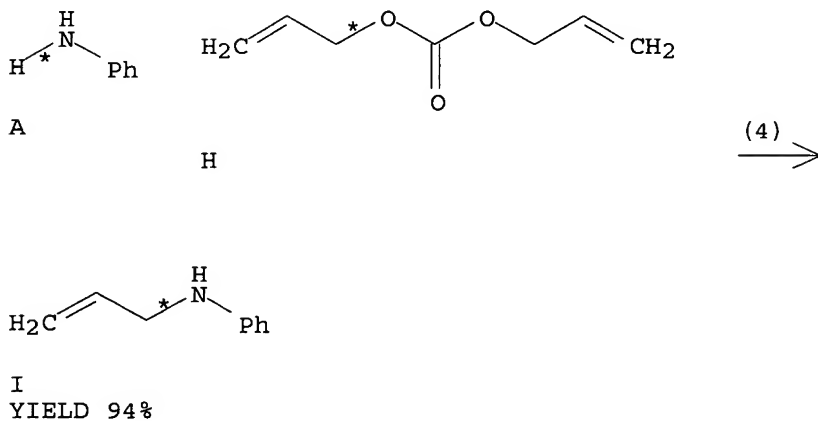
RX(2) RCT A 62-53-3, D 105-58-8
 PRO E 103-69-5
 NTE NaY faujasite catalyst used; no solvent; thermal; green chem.-waste redn.

RX(3) OF 12 A + F ==> G



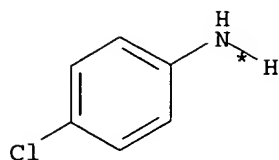
RX(3) RCT A 62-53-3, F 3459-92-5
 PRO G 103-32-2
 NTE NaY faujasite catalyst used; no solvent; thermal; green chem.-waste redn.

RX(4) OF 12 A + H ==> I

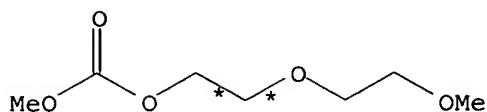


RX(4) RCT A 62-53-3, H 15022-08-9
 PRO I 589-09-3
 NTE NaY faujasite catalyst used; no solvent; thermal; green chem.-waste redn.

RX(5) OF 12 2 J + 3 B ==> K + L

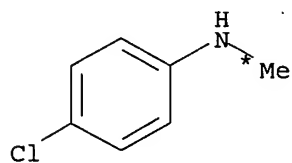
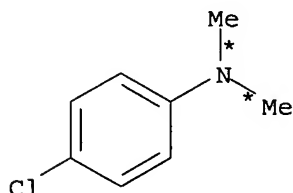


2 J



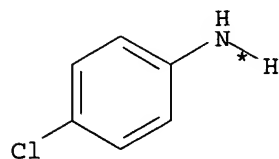
3 B

(5)

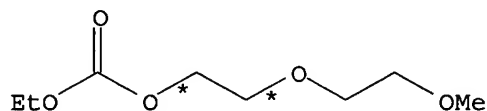
K
YIELD 75%L
YIELD 5%

RX(5) RCT J 106-47-8, B 141814-27-9
 PRO K 932-96-7, L 698-69-1
 NTE NaY faujasite catalyst used; no solvent; thermal;
 regioselective; green chem.-waste redn.

RX(6) OF 12 J + M ==> N

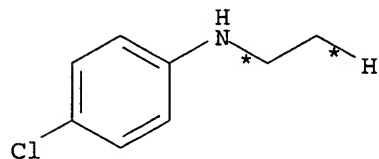


J



M

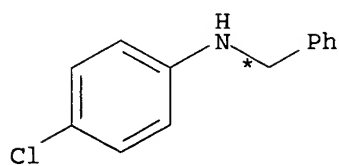
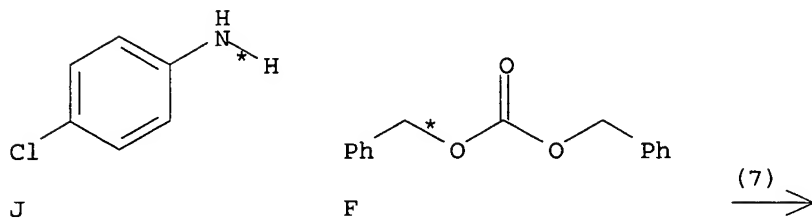
(6)

N
YIELD 82%

RX(6) RCT J 106-47-8, M 214470-03-8
 PRO N 13519-75-0
 NTE NaY faujasite catalyst used; no solvent; thermal;

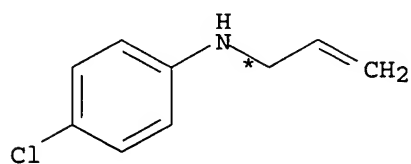
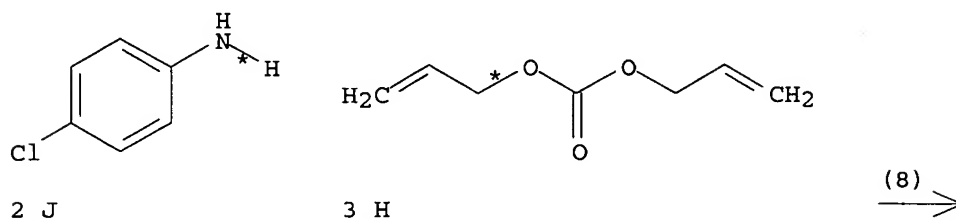
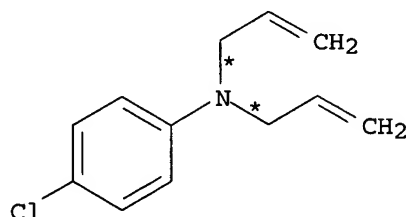
regioselective; green chem.-waste redn.

RX(7) OF 12 J + F ==> O

O
YIELD 70%

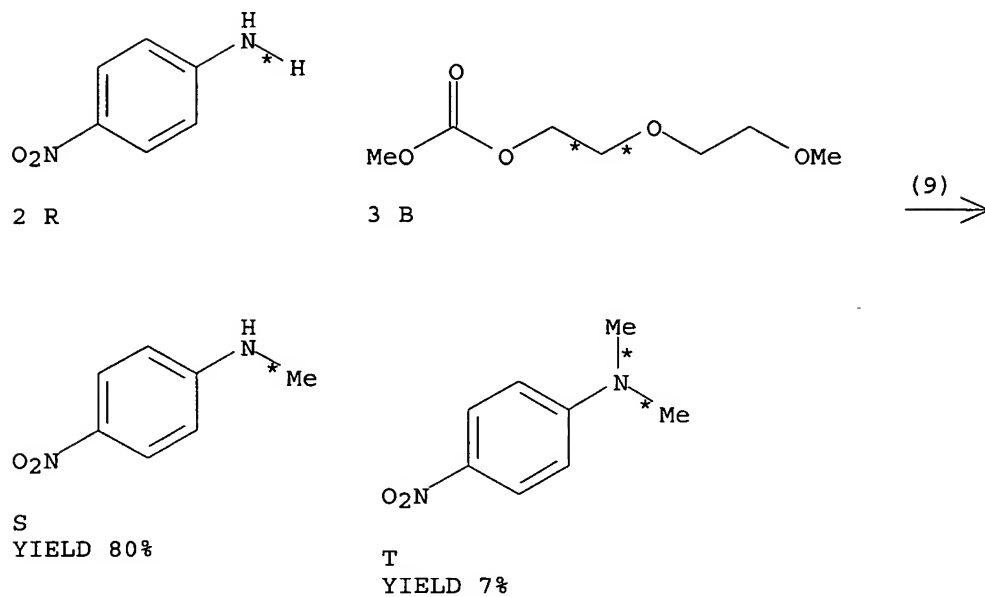
RX(7) RCT J 106-47-8, F 3459-92-5
 PRO O 2948-37-0
 NTE NaY faujasite catalyst used; no solvent; thermal; green
 chem.-waste redn.

RX(8) OF 12 2 J + 3 H ==> P + Q

P
YIELD 82%Q
YIELD 5%

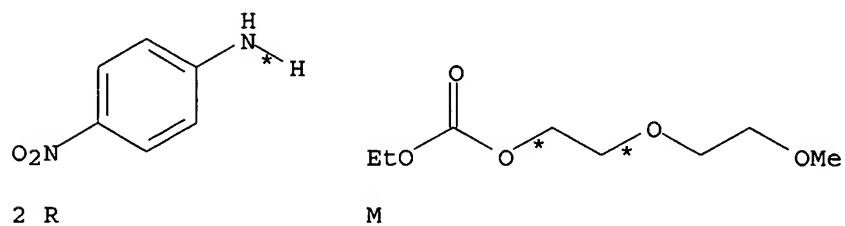
RX(8) RCT J 106-47-8, H 15022-08-9
 PRO P 13519-80-7, Q 30438-94-9
 NTE NaY faujasite catalyst used; no solvent; thermal; green
 chem.-waste redn.

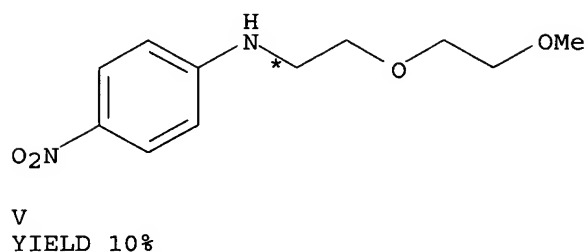
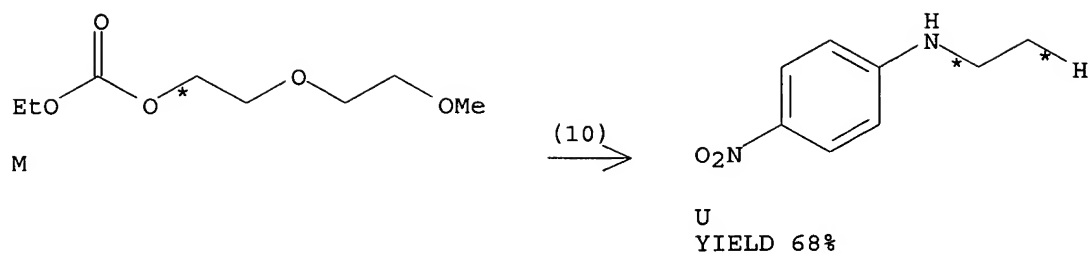
RX(9) OF 12 2 R + 3 B ==> S + T



RX(9) RCT R 100-01-6, B 141814-27-9
 PRO S 100-15-2, T 100-23-2
 NTE NaY faujasite catalyst used; no solvent; thermal;
 regioselective; green chem.-waste redn.

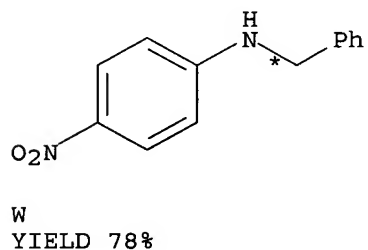
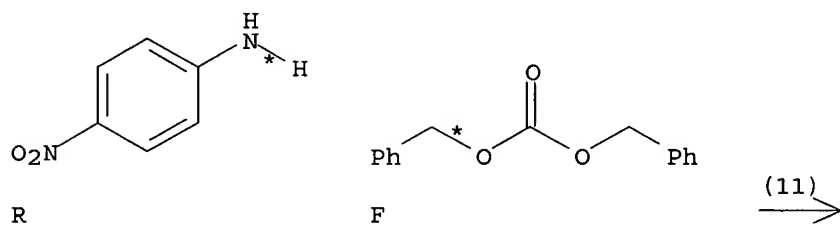
RX(10) OF 12 2 R + 2 M ==> U + V





RX(10) RCT R 100-01-6, M 214470-03-8
 PRO U 3665-80-3, V 329767-78-4
 NTE NaY faujasite catalyst used; no solvent; thermal;
 regioselective; green chem.-waste redn.

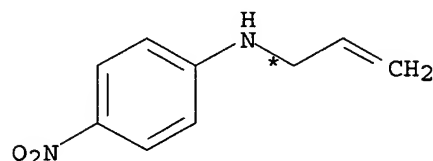
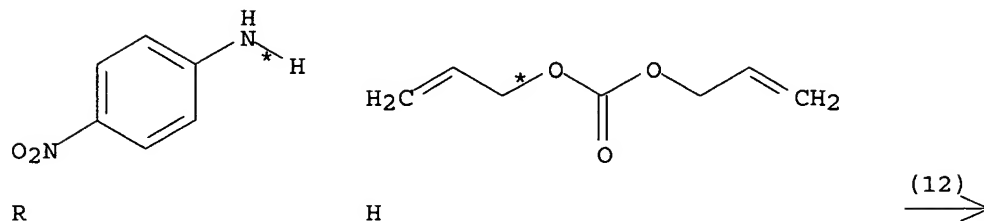
RX(11) OF 12 R + F ==> W



RX(11) RCT R 100-01-6, F 3459-92-5
 PRO W 14309-92-3

NTE NaY faujasite catalyst used; no solvent; thermal; green chem.-waste redn.

RX(12) OF 12 R + H ==> X



YIELD 78%

RX(12) RCT R 100-01-6, H 15022-08-9

PRO X 4138-40-3

NTE NaY faujasite catalyst used; no solvent; thermal; green chem.-waste redn.

AU Selva, Maurizio; Tundo, Pietro; Perosa, Alvise

L61 ANSWER 3 OF 9 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 142:463238 CASREACT

TITLE: Mono-N-methylation of Functionalized Anilines with Alkyl Methyl Carbonates over NaY Faujasites. 4. Kinetics and Selectivity

AUTHOR(S): Selva, Maurizio; Tundo, Pietro; Foccardi, Tommaso

CORPORATE SOURCE: Dipartimento di Scienze Ambientali, Universita Ca' Foscari, Venice, 30123, Italy

SOURCE: Journal of Organic Chemistry (2005), 70(7), 2476-2485 CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

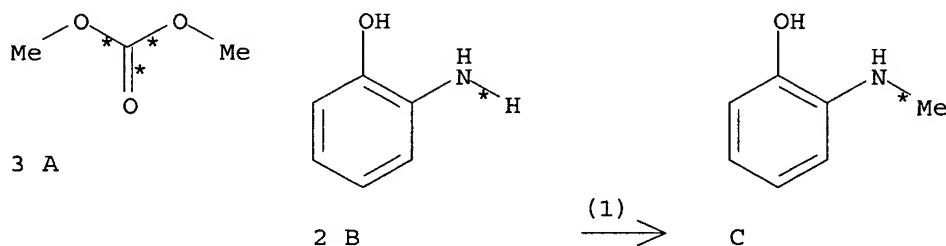
LANGUAGE: English

AB In the presence of NaY faujasite as the catalyst, the reaction of bifunctional anilines (1-4: XC6H4NH2; X = OH, CO2H, CH2OH, and CONH2) with Me alkyl carbonates [MeOCO2R': R' = Me or MeO(CH2)2O(CH2)2] proceeds with a very high mono-N-Me selectivity (XC6H4NHMe up to 99%), and chemoselectivity as well, with other nucleophilic functions (OH, CO2H, CH2OH, CONH2) fully preserved from alkylation and/or transesterification reactions. Aromatic substituents, however, modify the relative reactivity of amines 1-4: good evidence suggests that, not only steric and electronic effects, but, importantly, direct acid-base interactions between

substituents and the catalyst are involved. Weakly acidic groups (OH, CH₂OH, CONH₂, pK_a ≥ 10) may help the reaction, while aminobenzoic acids (pK_a of 4-5) are the least reactive substrates. The solvent polarity also affects the reaction, which is faster in xylene than in the more polar diglyme. The mono-N-Me selectivity is explained by the adsorption pattern of reagents within the zeolite pores: a BA12 displacement of the amine on Me alkyl carbonate should occur aided by the geometric features of the NaY supercavities. Different factors account for the reaction chemoselectivity. The polarizability of the two nucleophilic terms (NH₂ and X groups) of anilines is relevant, although adsorption and confinement phenomena of reagents promoted by the zeolite should also be considered.

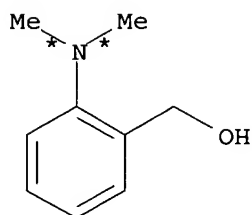
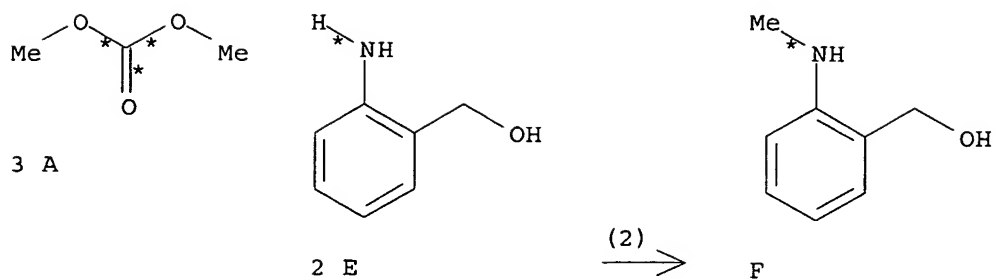
REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(1) OF 21 3 A + 2 B ==> C + D



RX(1) RCT A 616-38-6, B 95-55-6
 PRO C 611-24-5, D 3743-22-4
 SOL 616-38-6 Me₂CO₃
 CON 150 minutes, 90 deg C
 NTE chemoselective, solid-supported catalyst, kinetic study, NaY Faujasite catalyst used, selective to mono-N-methylation, alternate preparation described

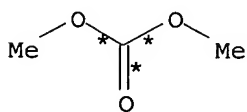
RX(2) OF 21 3 A + 2 E ==> F + G



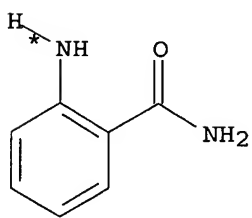
G

RX(2) RCT A 616-38-6, E 5344-90-1
 PRO F 29055-08-1, G 4707-56-6
 SOL 616-38-6 Me₂CO₃
 CON 405 minutes, 90 deg C
 NTE chemoselective, solid-supported catalyst, kinetic study, NaY
 Faujasite catalyst used, selective to mono-N-methylation,
 alternate preparation described

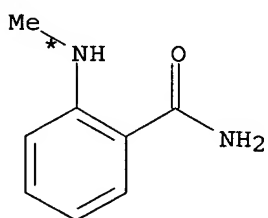
RX(3) OF 21 3 A + 2 H ==> I + J



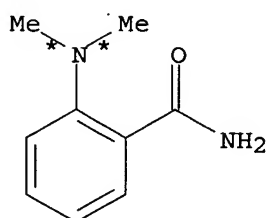
3 A



2 H



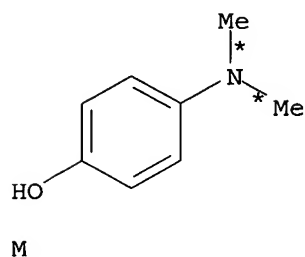
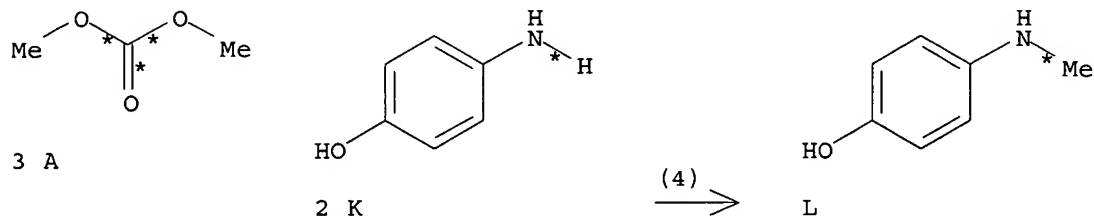
I



J

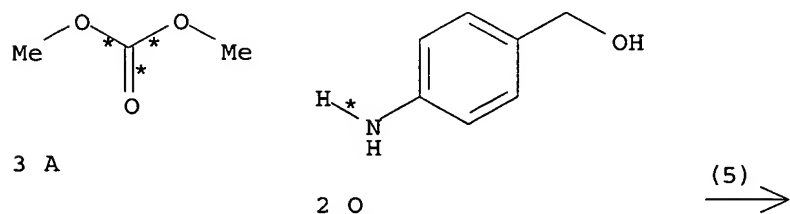
RX(3) RCT A 616-38-6, H 88-68-6
 PRO I 7505-81-9, J 56042-77-4
 SOL 616-38-6 Me₂CO₃
 CON 540 minutes, 90 deg C
 NTE regioselective, solid-supported catalyst, kinetic study, NaY
 Faujasite catalyst used, selective to mono-N-methylation,
 alternate preparation described

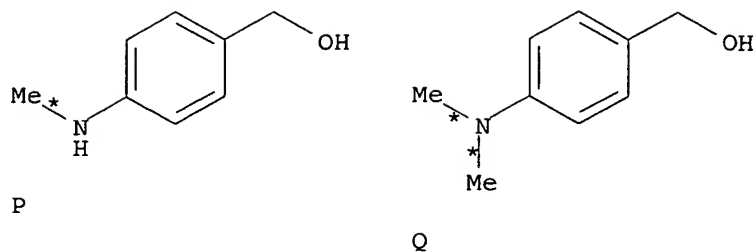
RX(4) OF 21 3 A + 2 K ==> L + M



RX(4) RCT A 616-38-6, K 123-30-8
 PRO L 150-75-4, M 619-60-3
 SOL 616-38-6 Me₂CO₃, 110-71-4 (CH₂OMe)₂
 CON 315 minutes, 84 deg C
 NTE chemoselective, solid-supported catalyst, kinetic study, NaY
 Faujasite catalyst used, selective to mono-N-methylation,
 alternate preparation described

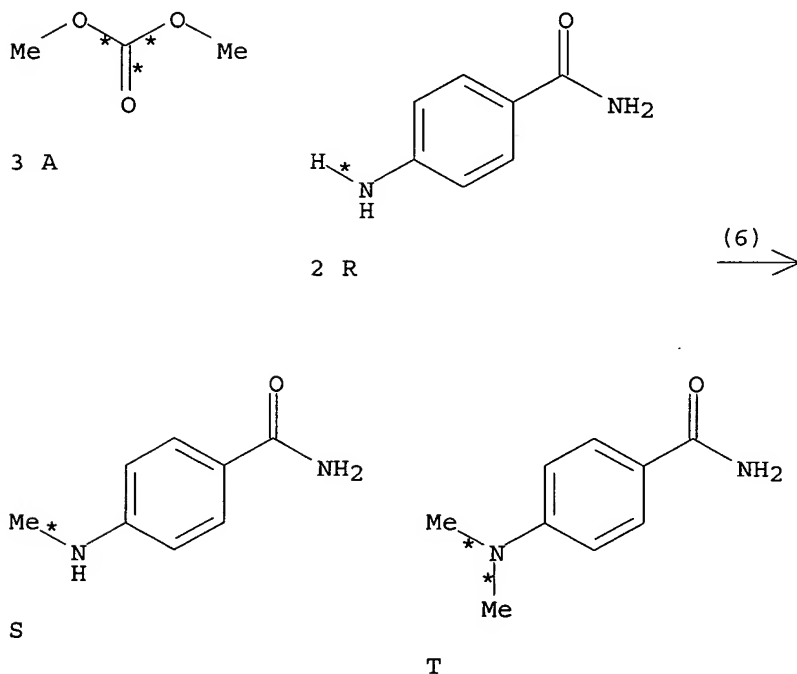
RX(5) OF 21 3 A + 2 O ==> P + Q





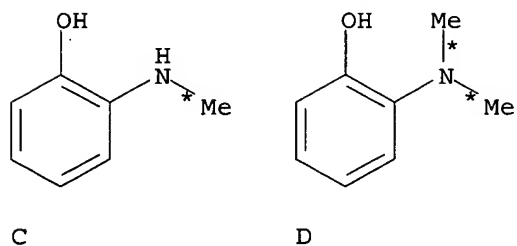
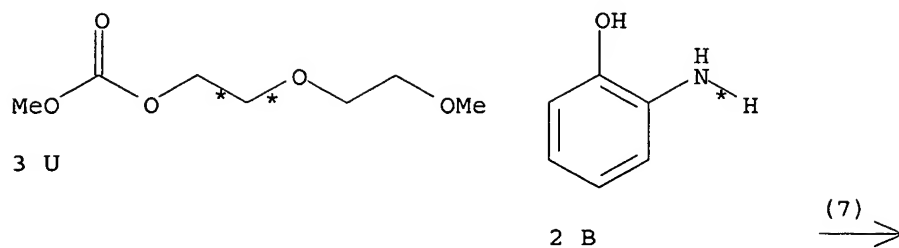
RX(5) RCT A 616-38-6, O 623-04-1
 PRO P 181819-75-0, Q 1703-46-4
 SOL 616-38-6 Me2CO3, 110-71-4 (CH2OMe)2
 CON 570 minutes, 84 deg C
 NTE chemoselective, solid-supported catalyst, kinetic study, NaY
 Faujasite catalyst used, selective to mono-N-methylation,
 alternate preparation described

RX(6) OF 21 3 A + 2 R ==> S + T.



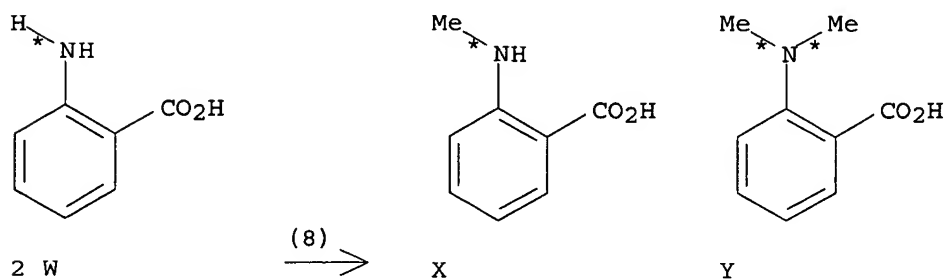
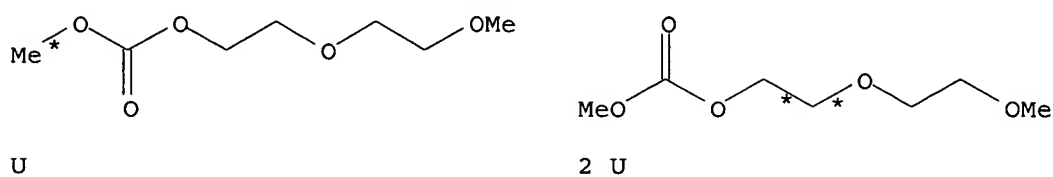
RX(6) RCT A 616-38-6, R 2835-68-9
 PRO S 38359-26-1, T 6083-47-2
 SOL 616-38-6 Me2CO3, 110-71-4 (CH2OMe)2
 CON 570 minutes, 84 deg C
 NTE regioselective, solid-supported catalyst, kinetic study, NaY
 Faujasite catalyst used, selective to mono-N-methylation,
 alternate preparation described

RX (7) OF 21 3 U + 2 B ==> C + D



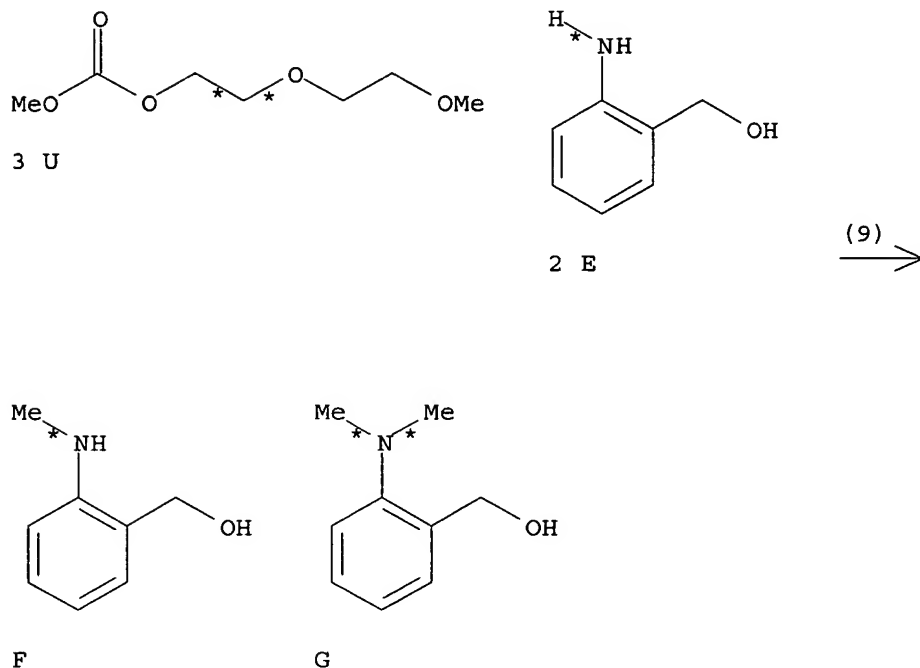
RX (7) RCT U 141814-27-9, B 95-55-6
 PRO C 611-24-5, D 3743-22-4
 SOL 1330-20-7 Xylene
 CON 10 minutes, 135 deg C
 NTE chemoselective, solid-supported catalyst, kinetic study, NaY
 Faujasite catalyst used, selective to mono-N-methylation,
 alternate preparation described

RX (8) OF 21 3 U + 2 W ==> X + Y



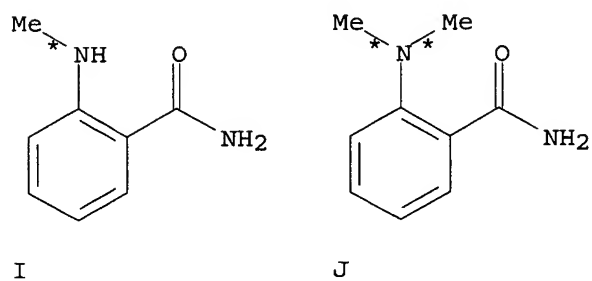
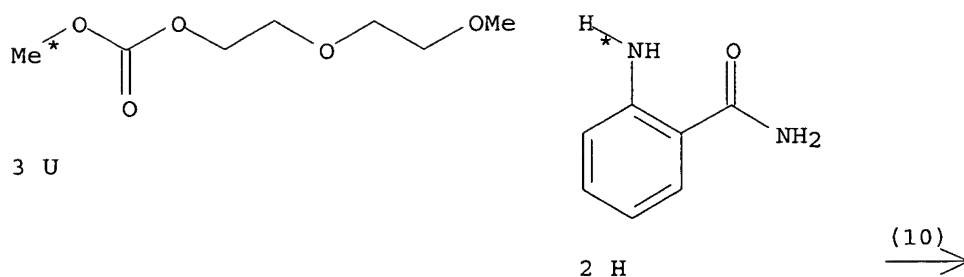
RX(8) RCT U 141814-27-9, W 118-92-3
 PRO X 119-68-6, Y 610-16-2
 SOL 1330-20-7 Xylene
 CON 540 minutes, 135 deg C
 NTE chemoselective, solid-supported catalyst, kinetic study, NaY
 Faujasite catalyst used, selective to mono-N-methylation,
 alternate preparation described

RX(9) OF 21 3 U + 2 E ==> F + G



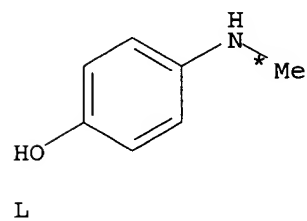
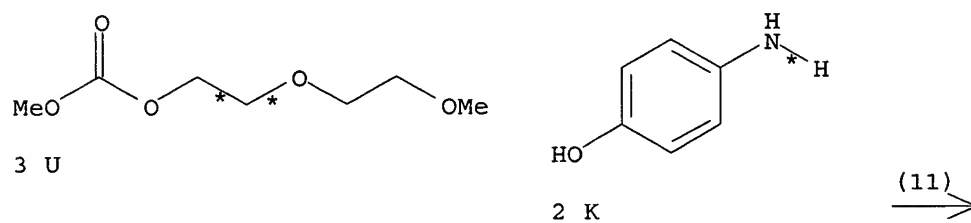
RX(9) RCT U 141814-27-9, E 5344-90-1
 PRO F 29055-08-1, G 4707-56-6
 SOL 1330-20-7 Xylene
 CON 80 minutes, 135 deg C
 NTE chemoselective, solid-supported catalyst, kinetic study, NaY
 Faujasite catalyst used, selective to mono-N-methylation,
 alternate preparation described

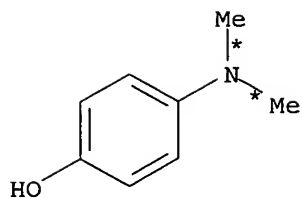
RX(10) OF 21 3 U + 2 H ==> I + J



RX(10) RCT U 141814-27-9, H 88-68-6
 PRO I 7505-81-9, J 56042-77-4
 SOL 1330-20-7 Xylene
 CON 80 minutes, 135 deg C
 NTE regioselective, solid-supported catalyst, kinetic study, NaY
 Faujasite catalyst used, selective to mono-N-methylation,
 alternate preparation described

RX(11) OF 21 3 U + 2 K ==> L + M

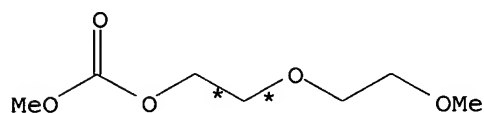




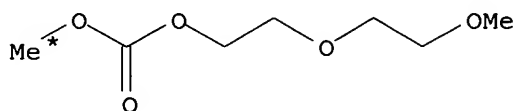
M

RX(11) RCT U 141814-27-9, K 123-30-8
 PRO L 150-75-4, M 619-60-3
 SOL 111-96-6 (MeOCH₂CH₂)₂O
 CON 50 minutes, 135 deg C
 NTE chemoselective, solid-supported catalyst, kinetic study, NaY
 Faujasite catalyst used, selective to mono-N-methylation,
 alternate preparation described

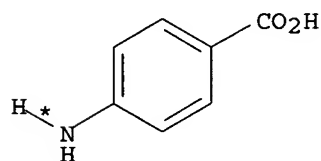
RX(12) OF 21 3 U + 2 AA ==> AB + AC



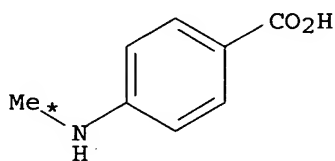
2 U



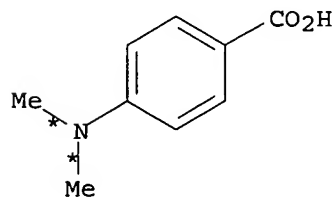
U



2 AA



AB

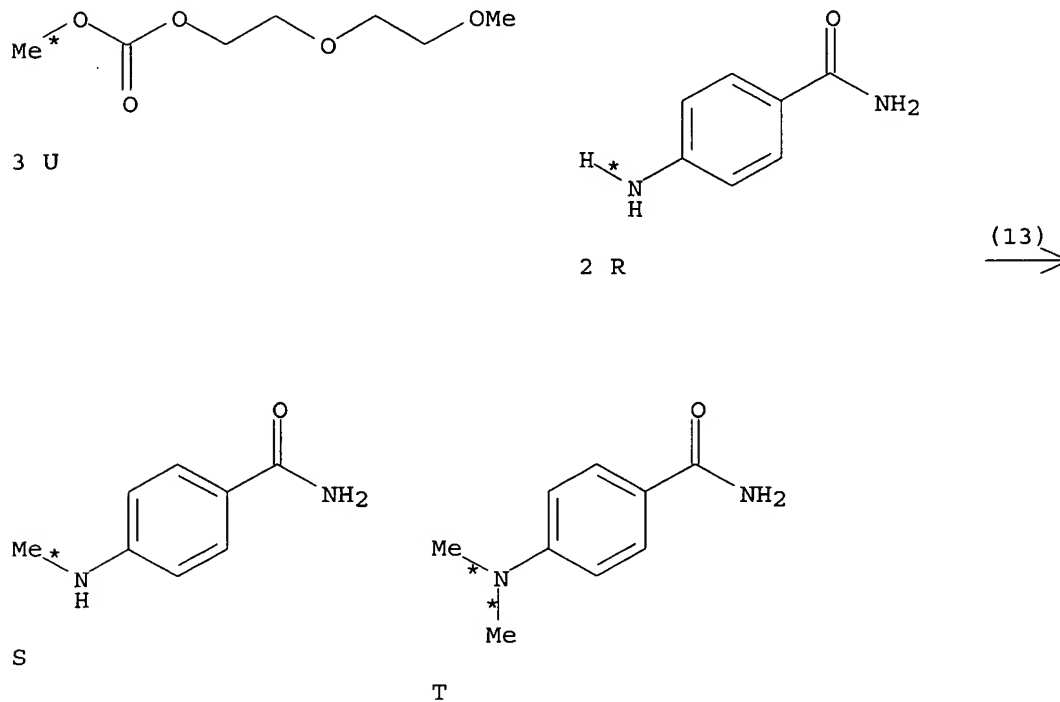


AC

RX(12) RCT U 141814-27-9, AA 150-13-0
 PRO AB 10541-83-0, AC 619-84-1
 SOL 111-96-6 (MeOCH₂CH₂)₂O
 CON 600 minutes, 135 deg C

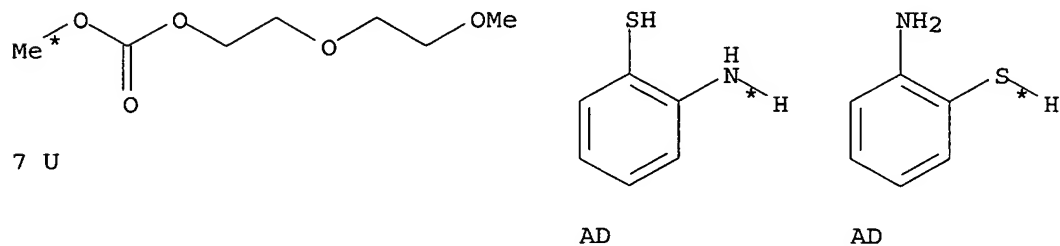
NTE chemoselective, solid-supported catalyst, kinetic study, NaY
Faujasite catalyst used, selective to mono-N-methylation

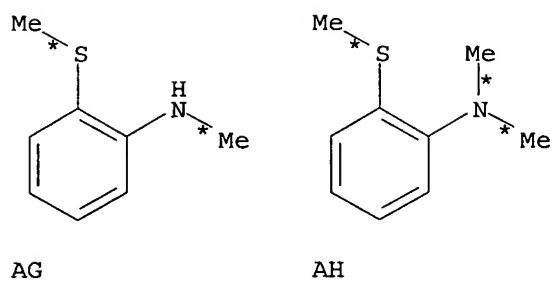
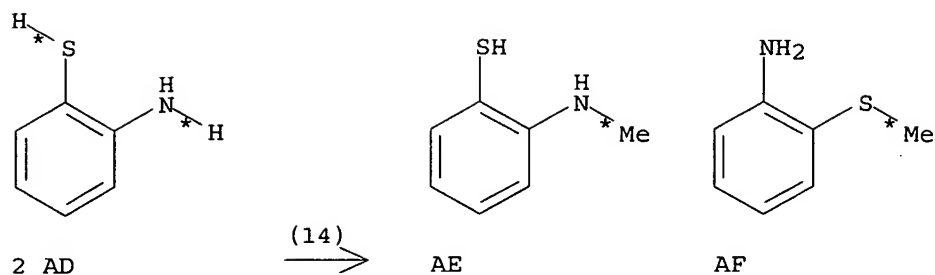
RX(13) OF 21 3 U + 2 R ==> S + T



RX(13) RCT U 141814-27-9, R 2835-68-9
 PRO S 38359-26-1, T 6083-47-2
 SOL 111-96-6 (MeOCH₂CH₂)₂O
 CON 50 minutes, 135 deg C
 NTE regioselective, solid-supported catalyst, kinetic study, NaY
 Faujasite catalyst used, selective to mono-N-methylation,
 alternate preparation described

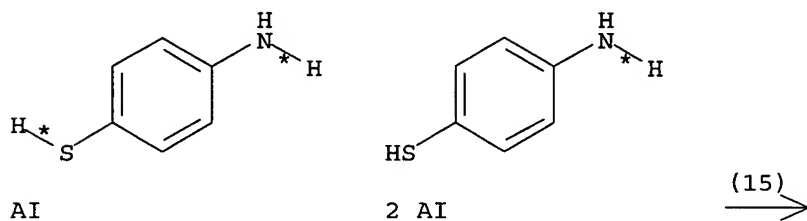
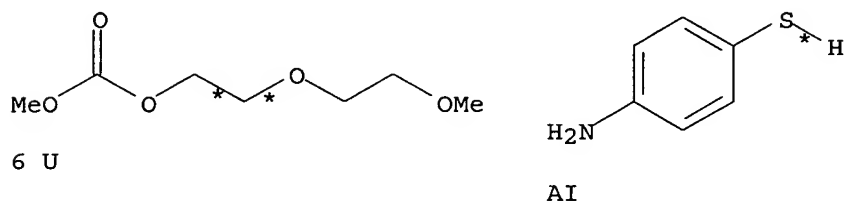
RX(14) OF 21 7 U + 4 AD ==> AE + AF +
 AG + AH

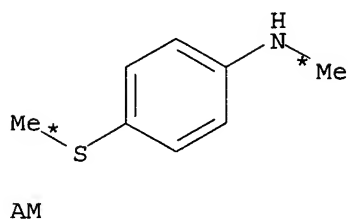
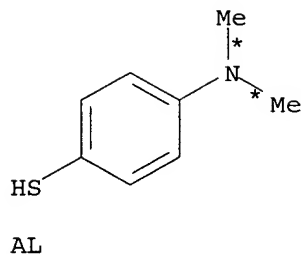
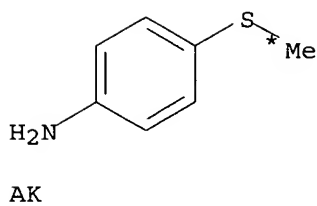
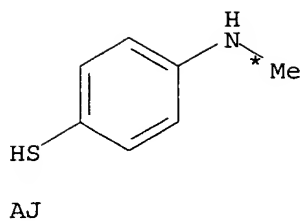




RX(14) RCT U 141814-27-9, AD 137-07-5
 PRO AE 21749-63-3, AF 2987-53-3, AG 13372-62-8, AH 2388-50-3
 SOL 1330-20-7 Xylene
 CON 8 hours, 135 deg C
 NTE chemoselective, solid-supported catalyst, kinetic study, NaY Faujasite catalyst used

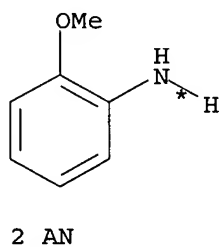
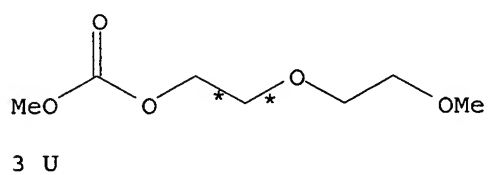
RX(15) OF 21 6 U + 4 AI ==> AJ + AK +
 AL + AM



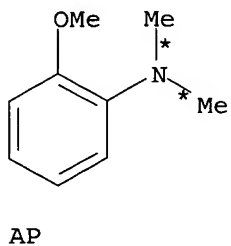
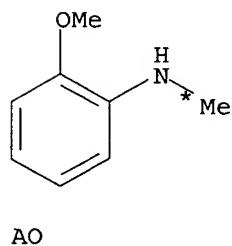


RX(15) RCT U 141814-27-9, AI 1193-02-8
 PRO AJ 4946-21-8, AK 104-96-1, AL 4946-22-9, AM 58259-33-9
 SOL 1330-20-7 Xylene
 CON 4 hours, 135 deg C
 NTE chemoselective, solid-supported catalyst, kinetic study, NaY
 Faujasite catalyst used

RX(16) OF 21 3 U + 2 AN ==> AO + AP

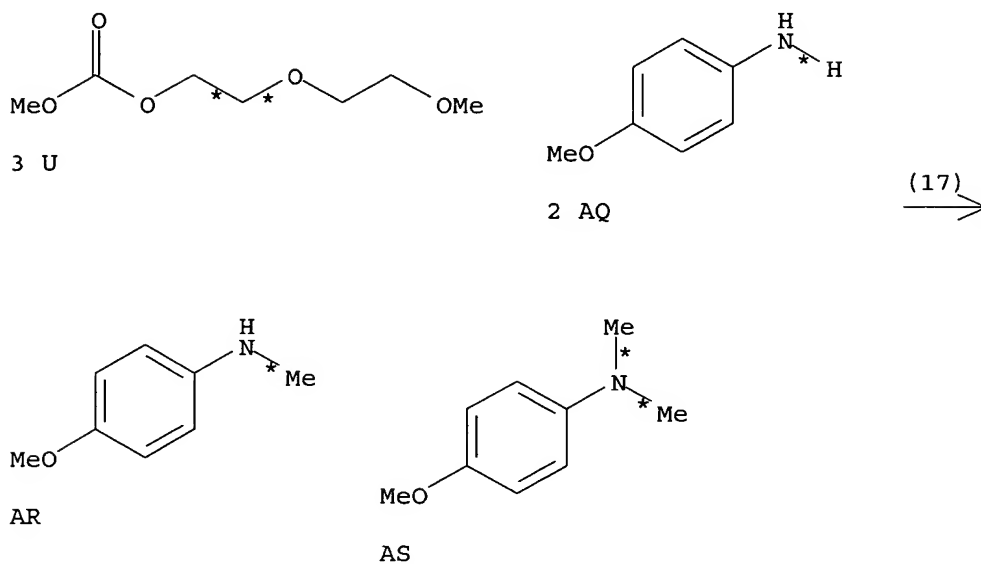


(16) →



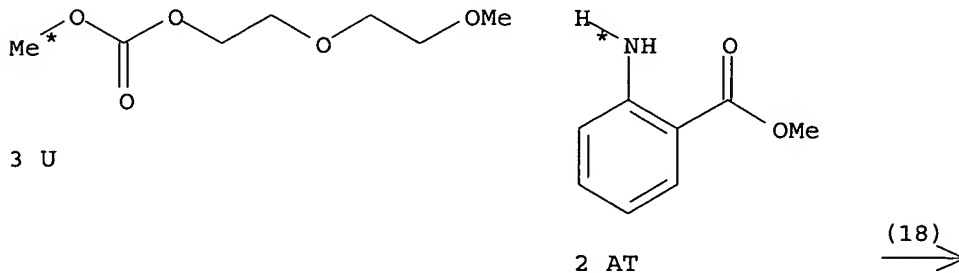
RX(16) RCT U 141814-27-9, AN 90-04-0
 PRO AO 10541-78-3, AP 700-75-4
 SOL 1330-20-7 Xylene
 CON 1320 minutes, 135 deg C
 NTE solid-supported catalyst, kinetic study, NaY Faujasite catalyst
 used, selective to mono-N-methylation

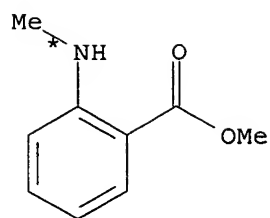
RX(17) OF 21 3 U + 2 AQ ==> AR + AS



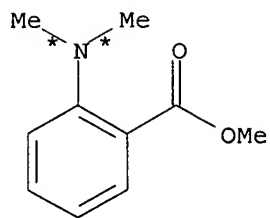
RX(17) RCT U 141814-27-9, AQ 104-94-9
 PRO AR 5961-59-1, AS 701-56-4
 SOL 1330-20-7 Xylene
 CON 210 minutes, 135 deg C
 NTE solid-supported catalyst, kinetic study, NaY Faujasite catalyst
 used, selective to mono-N-methylation

RX(18) OF 21 3 U + 2 AT ==> AU + AV





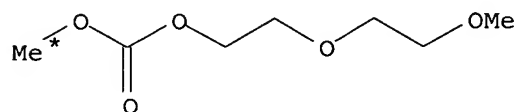
AU



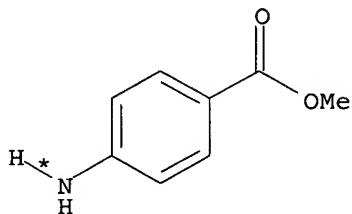
AV

RX (18) RCT U 141814-27-9, AT 134-20-3
 PRO AU 85-91-6, AV 10072-05-6
 SOL 1330-20-7 Xylene
 CON 660 minutes, 135 deg C
 NTE solid-supported catalyst, kinetic study, NaY Faujasite catalyst
 used, selective to mono-N-methylation

RX (19) OF 21 3 U + 2 AW ==> AX + AY

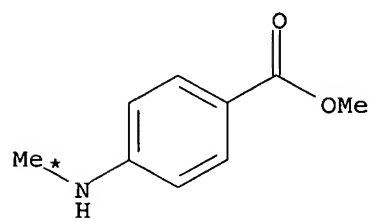


3 U

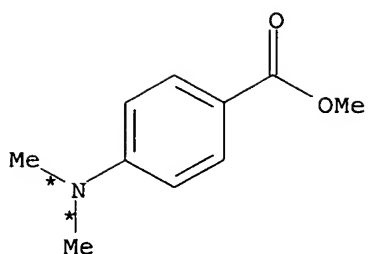


2 AW

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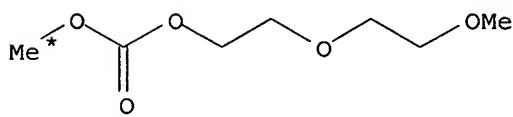
AX



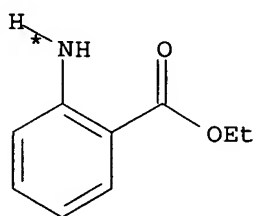
AY

RX(19) RCT U 141814-27-9, AW 619-45-4
 PRO AX 18358-63-9, AY 1202-25-1
 SOL 1330-20-7 Xylene
 CON 270 minutes, 135 deg C
 NTE solid-supported catalyst, kinetic study, NaY Faujasite catalyst
 used, selective to mono-N-methylation

RX(20) OF 21 3 U + 2 AZ ==> BA + BB

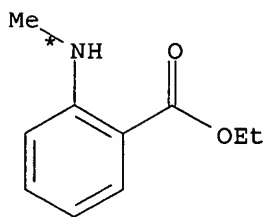


3 U

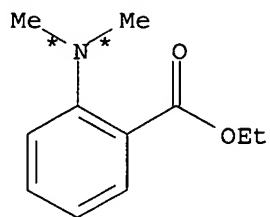


2 AZ

(20) →



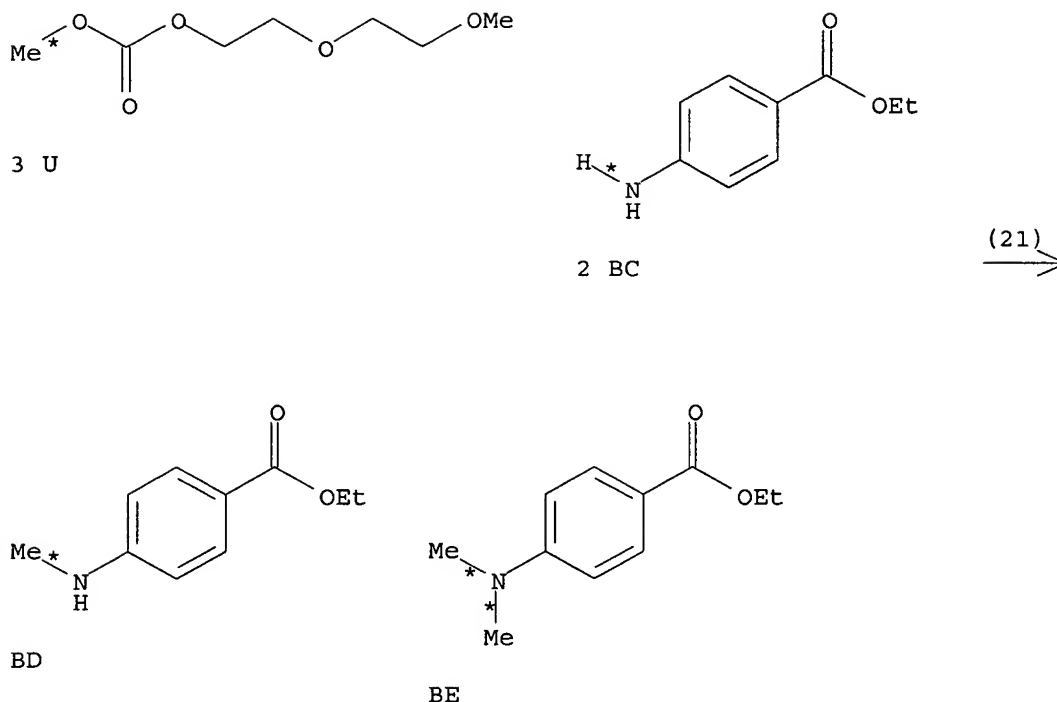
BA



BB

RX(20) RCT U 141814-27-9, AZ 87-25-2
 PRO BA 35472-56-1, BB 55426-74-9
 SOL 1330-20-7 Xylene
 CON 4680 minutes, 135 deg C
 NTE solid-supported catalyst, kinetic study, NaY Faujasite catalyst
 used, selective to mono-N-methylation

RX(21) OF 21 3 U + 2 BC ==> BD + BE



RX(21) RCT U 141814-27-9, BC 94-09-7
 PRO BD 10541-82-9, BE 10287-53-3
 SOL 1330-20-7 Xylene
 CON 540 minutes, 135 deg C
 NTE solid-supported catalyst, kinetic study, NaY Faujasite catalyst
 used, selective to mono-N-methylation
 AU Selva, Maurizio; Tundo, Pietro; Foccardi, Tommaso

L61 ANSWER 4 OF 9 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 142:335922 CASREACT

TITLE: Dimethyl Carbonate as an Ambident Electrophile

AUTHOR(S): Tundo, Pietro; Rossi, Laura; Loris, Alessandro

CORPORATE SOURCE: Dipartimento di Scienze Ambientali, Universita Ca' Foscari, Venice, Italy

SOURCE: Journal of Organic Chemistry (2005), 70(6), 2219-2224
CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

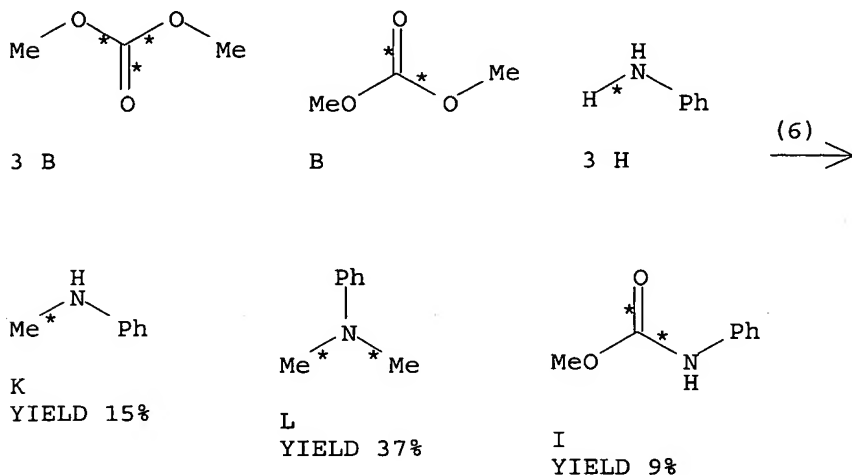
LANGUAGE: English

AB The features of various anions having different soft/hard character (aliphatic and aromatic amines, alkoxides, phenoxides, thiolates) are compared with regard to nucleophilic substitutions on di-Me carbonate (DMC), using different reaction conditions. Results are well in agreement with the Hard-Soft Acid-Base (HSAB) theory. Accordingly, the high selectivity of monomethylation of CH₂ acidic compds. and primary aromatic amines with DMC can be explained by two different subsequent reactions, which are due to the double electrophilic character of DMC. The first step consists of a hard-hard reaction and selectively produces a soft anion, which, in the

second phase, selectively transforms into the final monomethylated product, via a soft-soft nucleophilic displacement (yield >99% at complete conversion, using DMC as solvent).

REFERENCE COUNT: 42 THERE ARE 42 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(6) OF 17 4 B + 3 H ==> K + L + I



RX(6) RCT B 616-38-6, H 62-53-3
 PRO K 100-61-8, L 121-69-7, I 2603-10-3
 CON 24 hours, 200 deg C
 NTE chemoselective, high pressure
 AU Tundo, Pietro; Rossi, Laura; Loris, Alessandro

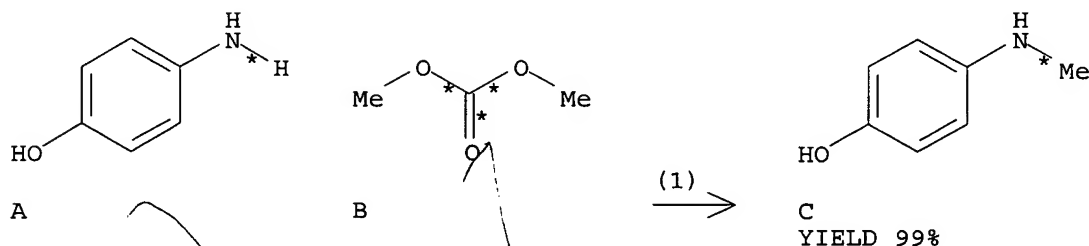
L61 ANSWER 5 OF 9 CASREACT COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 139:323290 CASREACT
 TITLE: Reaction of Functionalized Anilines with Dimethyl Carbonate over NaY Faujasite. 3. Chemoselectivity toward Mono-N-methylation
 AUTHOR(S): Selva, Maurizio; Tundo, Pietro; Perosa, Alvise
 CORPORATE SOURCE: Dipartimento di Scienze Ambientali, Universita Ca' Foscari, Venice, 30123, Italy
 SOURCE: Journal of Organic Chemistry (2003), 68(19), 7374-7378
 CODEN: JOCEAH; ISSN: 0022-3263
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English

AB In the presence of NaY faujasite, di-Me carbonate (MeOCO₂Me, DMC) is a highly chemoselective methylating agent of functionalized anilines such as aminophenols, aminobenzyl alcs., aminobenzoic acids, and aminobenzamides. The reaction proceeds with the exclusive formation of N-methylanilines without any concurrent O-methylation or N-/O-methoxy carbonylation side processes. Particularly, only mono-N-Me derivs. [XC₆H₄(1:1)NHMe, X = o-, m-, and p-OH; o- and p-CH₂OH; o- and p-CO₂H; o- and p-CONH₂] are obtained with selectivity up to 99% and isolated yields of 74-99%. DMC, which usually promotes methylations only at T > 120 °C, is activated by (1:1)the zeolite catalyst and it reacts with all aniline compds. at 90

°C. Aminobenzoic acids require a higher reaction temperature
(≥130 °C).

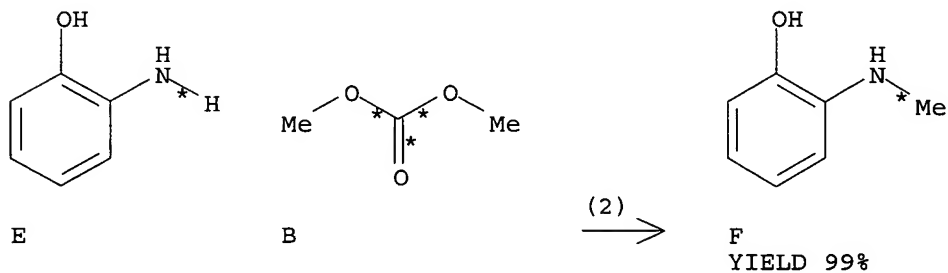
REFERENCE COUNT: 65 THERE ARE 65 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(1) OF 11 A + B ==> C



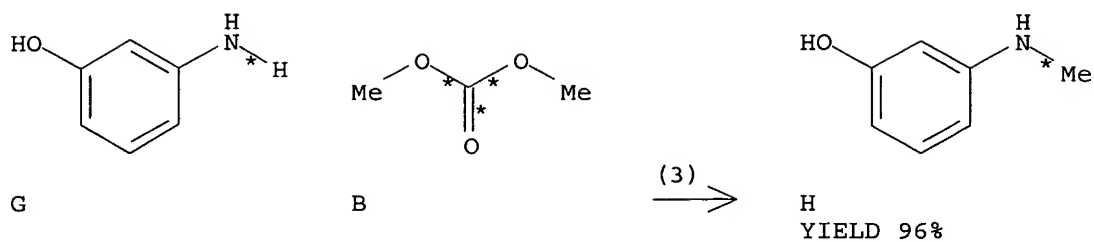
RX(1) RCT A 123-30-8, B 616-38-6
PRO C 150-75-4
SOL 75-05-8 MeCN
CON 24 hours, 81 deg C
NTE chemoselective, optimization study, NaY zeolite used

RX(2) OF 11 E + B ==> F



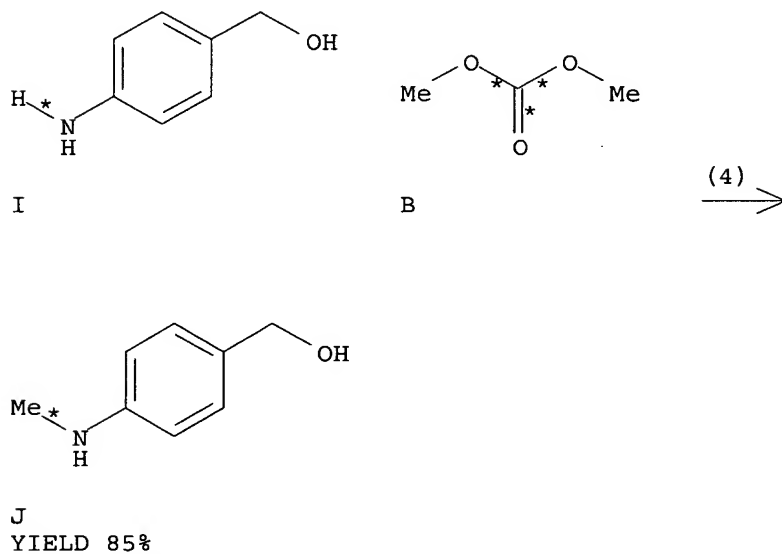
RX(2) RCT E 95-55-6, B 616-38-6
PRO F 611-24-5
SOL 616-38-6 Me2CO3
CON 3 hours, 90 deg C
NTE chemoselective, optimization study, NaY zeolite used

RX(3) OF 11 G + B ==> H



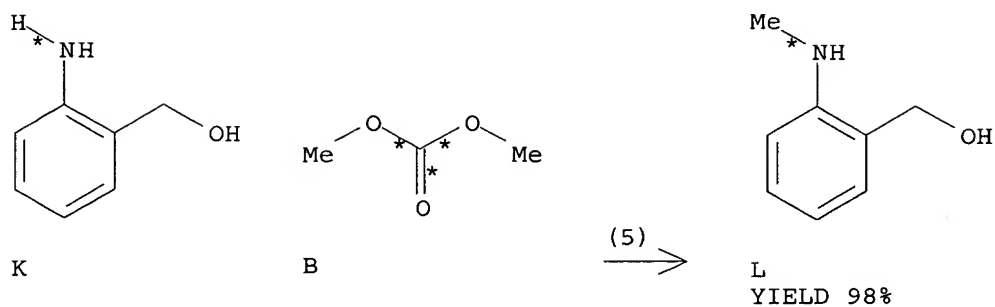
RX(3) RCT G 591-27-5, B 616-38-6
 PRO H 14703-69-6
 SOL 616-38-6 Me₂CO₃
 CON 3 hours, 90 deg C
 NTE chemoselective, NaY zeolite used

RX(4) OF 11 I + B ==> J



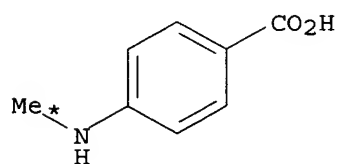
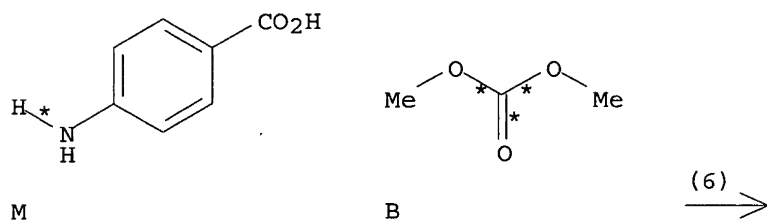
RX(4) RCT I 623-04-1, B 616-38-6
 PRO J 181819-75-0
 SOL 616-38-6 Me₂CO₃
 CON 8 hours, 90 deg C
 NTE chemoselective, NaY zeolite used

RX(5) OF 11 K + B ==> L



RX(5) RCT K 5344-90-1, B 616-38-6
 PRO L 29055-08-1
 SOL 616-38-6 Me₂CO₃
 CON 12 hours, 130 deg C
 NTE chemoselective, NaY zeolite used

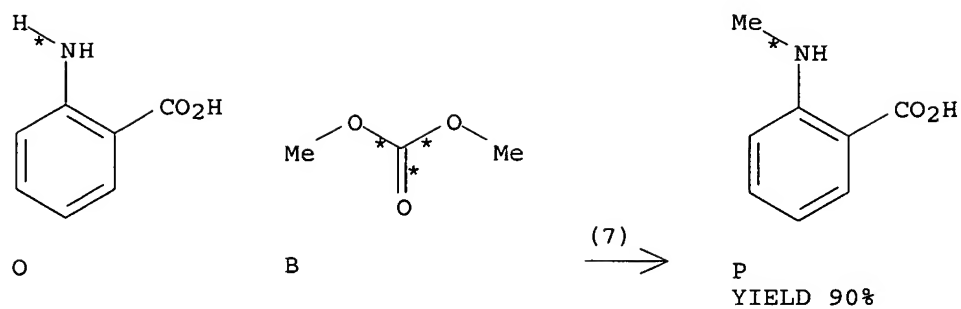
RX(6) OF 11 M + B ==> N



N
 YIELD 90%

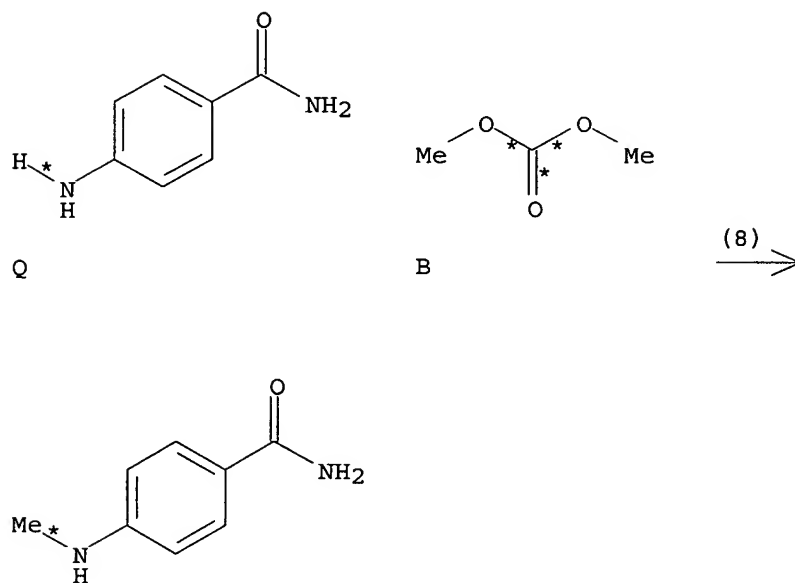
RX(6) RCT M 150-13-0, B 616-38-6
 PRO N 10541-83-0
 SOL 616-38-6 Me₂CO₃
 CON 9 hours, 90 deg C
 NTE chemoselective, NaY zeolite used

RX(7) OF 11 O + B ==> P



RX (7) RCT O 118-92-3, B 616-38-6
 PRO P 119-68-6
 SOL 616-38-6 Me₂CO₃
 CON 5 hours, 150 deg C
 NTE chemoselective, NaY zeolite used

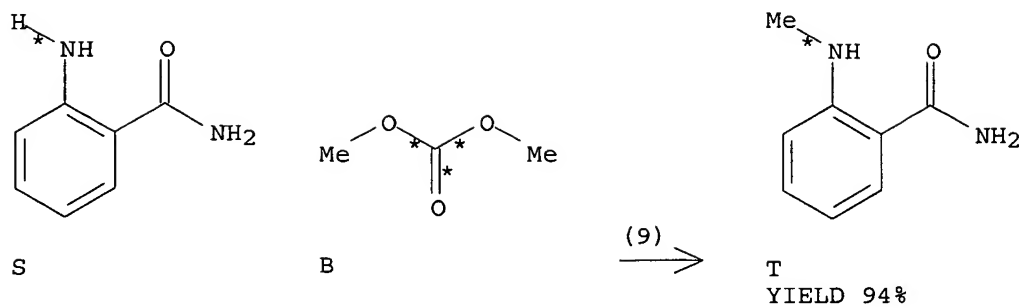
RX (8) OF 11 Q + B ==> R



R
YIELD 89%

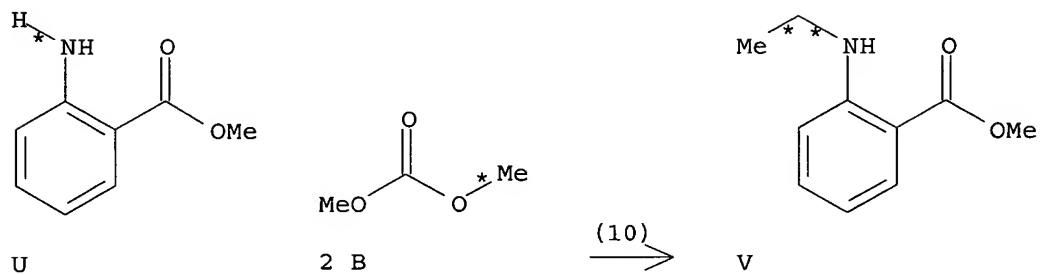
RX (8) RCT Q 2835-68-9, B 616-38-6
 PRO R 38359-26-1
 SOL 616-38-6 Me₂CO₃
 CON 24 hours, 90 deg C
 NTE chemoselective, NaY zeolite used

RX (9) OF 11 S + B ==> T



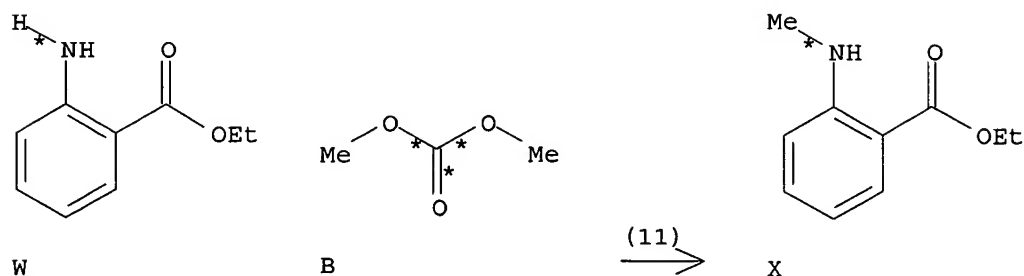
RX(9) RCT S 88-68-6, B 616-38-6
 PRO T 7505-81-9
 SOL 616-38-6 Me₂CO₃
 CON 22 hours, 90 deg C
 NTE chemoselective, NaY zeolite used

RX(10) OF 11 U + 2 B ==> V



RX(10) RCT U 134-20-3, B 616-38-6
 PRO V 17318-49-9
 SOL 616-38-6 Me₂CO₃
 CON 5 hours, 150 deg C
 NTE chemoselective, NaY zeolite used

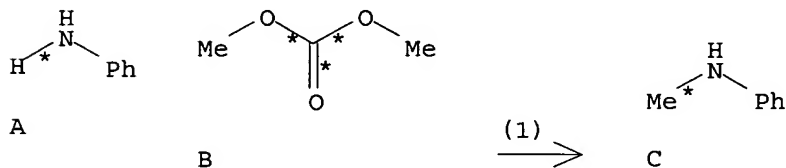
RX(11) OF 11 W + B ==> X



RX(11) RCT W 87-25-2, B 616-38-6
 PRO X 35472-56-1
 SOL 616-38-6 Me₂CO₃
 CON 5 hours, 150 deg C
 NTE chemoselective, NaY zeolite used
 AU Selva, Maurizio; Tundo, Pietro; Perosa, Alvise

L61 ANSWER 6 OF 9 CASREACT COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 111:25255 CASREACT
 TITLE: Gas-liquid phase-transfer catalysis: a new continuous-flow method in organic synthesis
 AUTHOR(S): Tundo, Pietro; Moraglio, Giovanni; Trotta, Francesco
 CORPORATE SOURCE: Ist. Chim. Ind., Univ. Messina, Messina, 98010, Italy
 SOURCE: Industrial & Engineering Chemistry Research (1989), 28(7), 881-90
 CODEN: IECRED; ISSN: 0888-5885
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB A new synthetic method, gas-liquid phase-transfer catalysis (GL-PTC), is described. GL-PTC is a continuous-flow procedure where gaseous reagents flow through a molten PT catalyst supported on a solid; no solvent is used. Reactions may develop through new mechanistic pathways compared with those of classical conditions; moreover, the reactions often occur in very selective ways. Some typical syntheses carried out under GL-PTC conditions are described in detail. They include syntheses of 2-alkylmalonic acid esters from the corresponding malonic acid esters, the reactions of Me₂CO₃, which give N-methylanilines from anilines and anisoles from phenols, and transesterification of EtOAc.

RX(1) OF 5 A + B ==> C

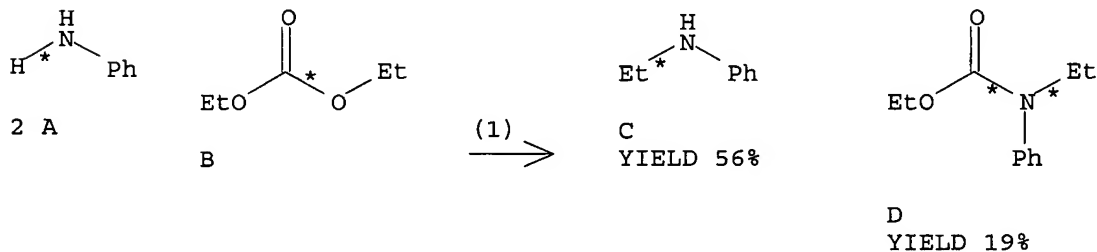


RX(1) RCT A 62-53-3, B 616-38-6
 PRO C 100-61-8
 AU Tundo, Pietro; Moraglio, Giovanni; Trotta, Francesco

L61 ANSWER 7 OF 9 CASREACT COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 106:155960 CASREACT
 TITLE: Selective mono-N-alkylation of aromatic amines by dialkyl carbonate under gas-liquid phase-transfer catalysis (GL-PTC) conditions
 AUTHOR(S): Trotta, F.; Tundo, P.; Moraglio, G.
 CORPORATE SOURCE: Ist. Chim. Org., Univ. Torino, Turin, 10125, Italy
 SOURCE: Journal of Organic Chemistry (1987), 52(7), 1300-4
 CODEN: JOCEAH; ISSN: 0022-3263
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB The reaction between aromatic amines and dialkyl carbonates, carried out in

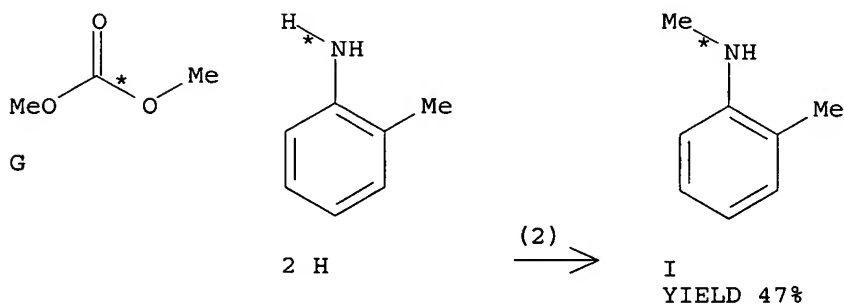
gas phase under GL-PTC conditions, in a continuous-flow process, produces the mono-N-alkylation product and its carboxyalkyl derivative with selectivity > 99%. The catalyst is a polyethylene glycol in the presence of K₂CO₃. The reaction produces CO₂, which is removed from the system, so that the reaction can be carried out indefinitely because the chemical nature of the catalytic bed, at steady state, does not change with time. The mechanism and selectivity were discussed.

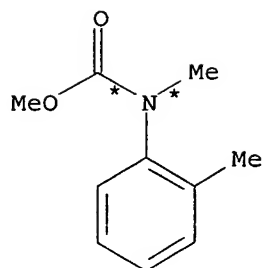
RX(1) OF 11 2 A + B ==> C + D



RX(1) RCT A 62-53-3, B 105-58-8
 RGT E 584-08-7 K₂CO₃
 PRO C 103-69-5, D 1013-75-8
 CAT 25322-68-3 HOCH₂CH₂OH polymer

RX(2) OF 11 G + 2 H ==> I + J

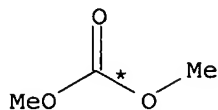




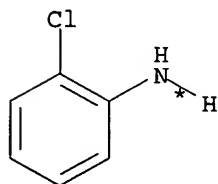
J
YIELD 25%

RX(2) RCT G 616-38-6, H 95-53-4
 RGT E 584-08-7 K2CO3
 PRO I 611-21-2, J 104189-18-6
 CAT 25322-68-3 HOCH2CH2OH polymer -

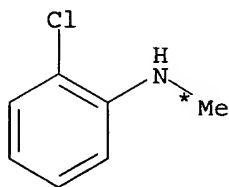
RX(3) OF 11 G + 2 K ==> L + M



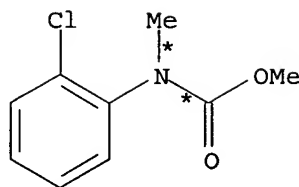
G



2 K



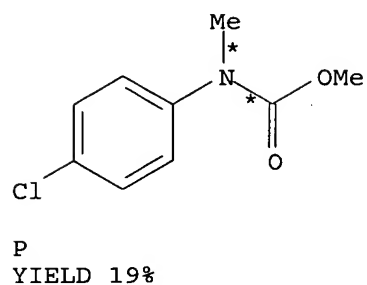
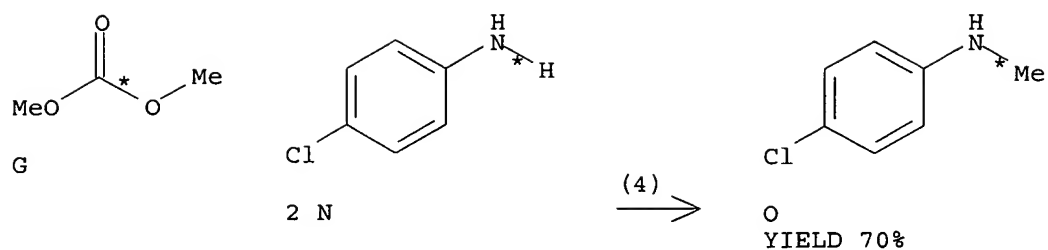
L
YIELD 62%



M
YIELD 22%

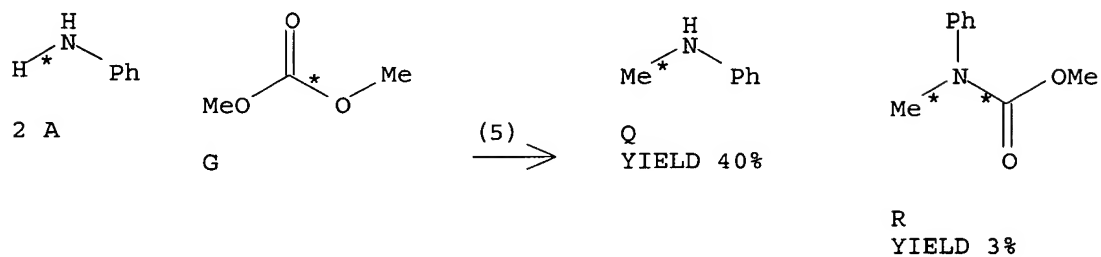
RX(3) RCT G 616-38-6, K 95-51-2
 RGT E 584-08-7 K2CO3
 PRO L 932-32-1, M 106712-21-4
 CAT 25322-68-3 HOCH2CH2OH polymer

RX(4) OF 11 G + 2 N ==> O + P



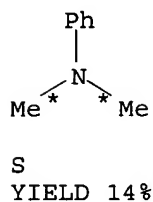
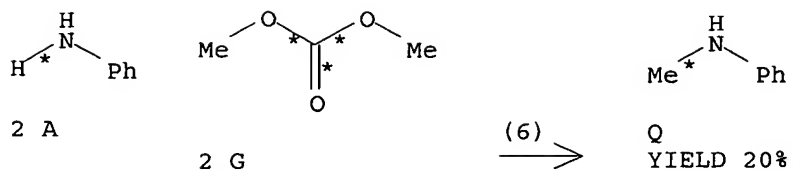
RX(4) RCT G 616-38-6, N 106-47-8
 RGT E 584-08-7 K₂CO₃
 PRO O 932-96-7, P 60561-39-9
 CAT 25322-68-3 HOCH₂CH₂OH polymer

RX(5) OF 11 2 A + G ==> Q + R



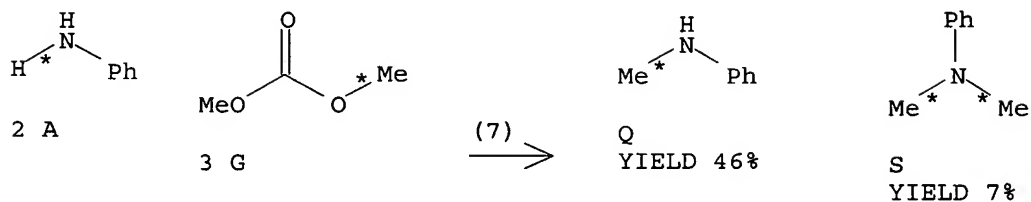
RX(5) RCT A 62-53-3, G 616-38-6
 RGT E 584-08-7 K₂CO₃
 PRO Q 100-61-8, R 28685-60-1
 CAT 25322-68-3 HOCH₂CH₂OH polymer

RX(6) OF 11 2 A + 2 G ==> Q + S



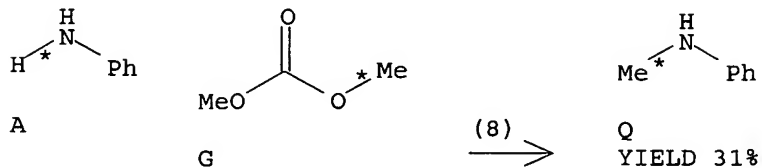
RX(6) RCT A 62-53-3, G 616-38-6
 PRO Q 100-61-8, S 121-69-7
 CAT 7631-86-9 SiO₂

RX(7) OF 11 2 A + 3 G ==> Q + S



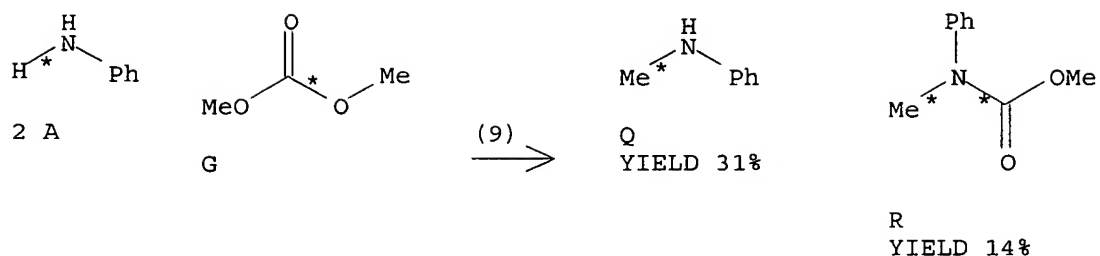
RX(7) RCT A 62-53-3, G 616-38-6
 PRO Q 100-61-8, S 121-69-7
 CAT 1344-28-1 Al₂O₃

RX(8) OF 11 A + G ==> Q



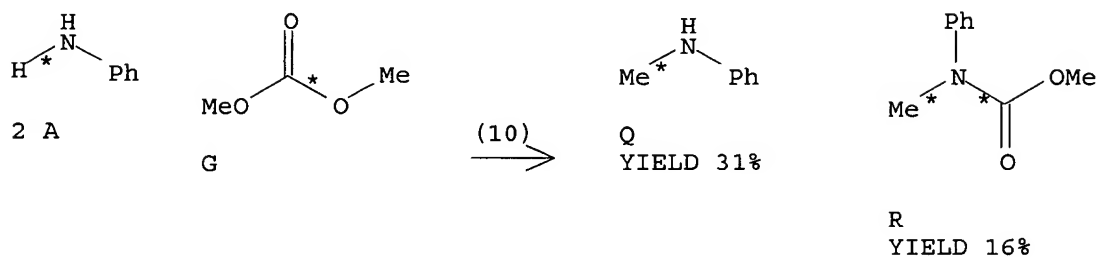
RX(8) RCT A 62-53-3, G 616-38-6
 RGT U 1344-28-1 Al₂O₃
 PRO Q 100-61-8
 CAT 3115-68-2 Bu₄P.Br

RX(9) OF 11 2 A + G ==> Q + R



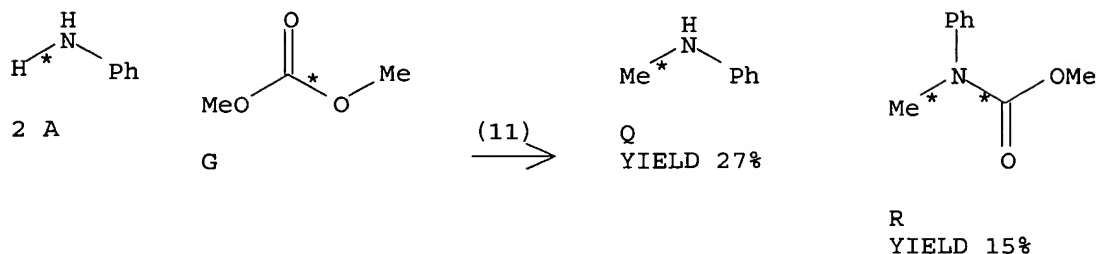
RX (9) RCT A 62-53-3, G 616-38-6
 RGT E 584-08-7 K₂CO₃
 PRO Q 100-61-8, R 28685-60-1
 CAT 25322-68-3 HOCH₂CH₂OH polymer
 SOL 110-82-7 Cyclohexane

RX (10) OF 11 2 A + G ==> Q + R



RX (10) RCT A 62-53-3, G 616-38-6
 RGT E 584-08-7 K₂CO₃
 PRO Q 100-61-8, R 28685-60-1
 CAT 25322-68-3 HOCH₂CH₂OH polymer
 SOL 109-99-9 THF

RX (11) OF 11 2 A + G ==> Q + R



RX (11) RCT A 62-53-3, G 616-38-6
 RGT E 584-08-7 K₂CO₃
 PRO Q 100-61-8, R 28685-60-1

CAT 25322-68-3 HOCH₂CH₂OH polymer
 SOL 123-91-1 Dioxane

AU Trotta, F.; Tundo, P.; Moraglio, G.

L61 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2002:894442 CAPLUS

DOCUMENT NUMBER: 138:106304

TITLE: Mono-N-methylation of Primary Amines with Alkyl Methyl Carbonates over Y Faujasites. 2. Kinetics and Selectivity

AUTHOR(S): Selva, Maurizio; Tundo, Pietro; Perosa, Alvise

CORPORATE SOURCE: Dipartimento di Scienze Ambientali, Universita Ca' Foscari, Venice, 30123, Italy

SOURCE: Journal of Organic Chemistry (2002), 67(26), 9238-9247
 CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB In the presence of a Na-exchanged Y faujasite, the reaction of primary aromatic amines 1 with 2-(2-methoxyethoxy)methylethyl **carbonate** [MeO(CH₂)₂O(CH₂)₂OCOMe, 2a] yields the corresponding mono-N-Me derivs. ArNHMe with selectivity up to 95%, at substantially quant. conversions. At 130 °C, the reaction can be run under diffusion-free conditions and is strongly affected by the solvent polarity: for instance, in going from xylene (ϵ_r = 2.40) to triglyme (ϵ_r = 7.62) as the solvent, the pseudo-first-order rate constant for the aniline (1a) disappearance shows a 5-fold decrease. In DMF (ϵ_r = 38.25), the same reaction does not occur at all. Competitive adsorption of the solvent and the substrate onto the catalytic sites accounts for this result. The behavior of alkyl-substituted anilines ZC₆H₄NH₂ [Z = p-Me, p-Et, p-Pr, p-(n-Bu) (1b-e); Z = 3,5-di-tert-butyl- and 2,4,6-tri-tert-butylanilines (1f,g)] and p-alkoxyanilines p-ZC₆H₄NH₂ [Z = OMe, OEt, OPr, O-n-Bu (1b'-e')] clearly indicates a steric effect of ring substituents: as diffusion of the amine into the catalytic pores is hindered, the reaction hardly proceeds and the mono-N-Me selectivity (SM/D) drops as well. Moreover, the strength of adsorption of the amine onto the catalyst influences the rate and the selectivity as well: the reaction of p-anisidine and p-toluidine - despite the higher nucleophilicity of these compds. - is slower and even less selective with respect to aniline. From a mechanistic viewpoint, the intermediacy of carbamates ArN(Me)CO₂R [R = MeO(CH₂)₂O(CH₂)₂] is suggested. At 90 °C, the reaction of benzylamine (7)-a model for aliphatic amines-with di-Me **carbonate** shows that the reaction outcome can be improved by tuning the amphoteric properties of the catalyst: in going from CsY to the more acidic LiY zeolite, methylation is not only more selective (SM/D ratio increases from 77% to 84%) but even much faster (CsY, conversion of 36% after 22 h; LiY, conversion of 43% after 7 h).

CC 22-4 (Physical Organic Chemistry)

ST amine methylation alkyl methyl **carbonate** faujasite catalyst kinetics selectivity

IT Y zeolites

RL: CAT (Catalyst use); USES (Uses)

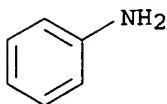
(CsY; kinetic study on mono-N-methylation of primary amines with alkyl Me carbonates over Y faujasites)

IT Faujasite-type zeolites

RL: CAT (Catalyst use); USES (Uses)

- (LiY; kinetic study on mono-N-methylation of primary amines with alkyl Me **carbonates** over Y **faujasites**)
- IT Y zeolites
RL: CAT (Catalyst use); USES (Uses)
(Na-exchanged; kinetic study on mono-N-methylation of primary amines with alkyl Me **carbonates** over Y **faujasites**)
- IT **Amines, reactions**
RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
(**aromatic**; kinetic study on mono-N-methylation of primary amines with alkyl Me **carbonates** over Y **faujasites**)
- IT Methylation catalysts
Methylation kinetics
Solvent polarity effect
Substituent effects
(kinetic study on mono-N-methylation of primary amines with alkyl Me **carbonates** over Y **faujasites**)
- IT Zeolite KY
RL: CAT (Catalyst use); USES (Uses)
(kinetic study on mono-N-methylation of primary amines with alkyl Me **carbonates** over Y **faujasites**)
- IT Dielectric constant
(of methoxyethoxymethylethyl **carbonate**; kinetic study on mono-N-methylation of primary amines with alkyl Me **carbonates** over Y **faujasites**)
- IT Methylation
(regioselective, of amines; kinetic study on mono-N-methylation of primary amines with alkyl Me **carbonates** over Y **faujasites**)
- IT 62-53-3, Aniline, reactions 100-46-9, Benzylamine, reactions 104-13-2, p-Butylaniline 104-94-9, p-Anisidine 106-49-0, p-Toluidine, reactions 156-43-4, p-Phenetidine 589-16-2, p-Ethylaniline 961-38-6, 2,4,6-Tri-tert-butylaniline 2380-36-1, 3,5-Di-tert-butylaniline 2696-84-6, p-Propylaniline 4344-55-2, 4-Butoxylaniline 4469-80-1, 4-Propoxyaniline 141814-27-9
RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
(kinetic study on mono-N-methylation of primary amines with alkyl Me **carbonates** over Y **faujasites**)
- IT 99-97-8 100-61-8, N-Methylaniline, formation (nonpreparative) 103-67-3 103-83-3 623-08-5 701-56-4 4150-37-2 5817-70-9 5961-59-1 37846-06-3 56475-82-2
RL: FMU (Formation, unclassified); FORM (Formation, nonpreparative)
(kinetic study on mono-N-methylation of primary amines with alkyl Me **carbonates** over Y **faujasites**)
- IT 1864-93-3 2909-79-7 3154-18-5 5279-59-4 13330-29-5 23563-27-1 36373-76-9 71089-15-1 137273-36-0 485795-30-0 485795-31-1 485795-32-2 485799-00-6
RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation, nonpreparative)
(kinetic study on mono-N-methylation of primary amines with alkyl Me **carbonates** over Y **faujasites**)
- IT 616-38-6, Dimethyl **carbonate**
RL: RCT (Reactant); RACT (Reactant or reagent)
(kinetic study on mono-N-methylation of primary amines with alkyl Me **carbonates** over Y **faujasites**)
- IT 68-12-2, DMF, uses 112-49-2, Triglyme 1330-20-7, Xylene, uses
RL: NUU (Other use, unclassified); USES (Uses)

(solvent; kinetic study on mono-N-methylation of primary amines with alkyl Me carbonates over Y faujasites)
 IT 62-53-3, Aniline, reactions
 RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent)
 (kinetic study on mono-N-methylation of primary amines with alkyl Me carbonates over Y faujasites)
 RN 62-53-3 CAPLUS
 CN Benzenamine (9CI) (CA INDEX NAME)



REFERENCE COUNT: 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L61 ANSWER 9 OF 9 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1997:271593 CAPLUS

DOCUMENT NUMBER: 127:17455

TITLE: Selective mono-N-methylation of primary aromatic amines by dimethyl carbonate over faujasite X- and Y-type zeolites

AUTHOR(S): Selva, Maurizio; Bomben, Andrea; Tundo, Pietro

CORPORATE SOURCE: Dip. Scienze Ambientali, Univ. Venezia, Venice, 2137-30123, Italy

SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1997), (7), 1041-1045

CODEN: JCPRB4; ISSN: 0300-922X

PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The reaction of di-Me carbonate (DMC) with different primary aromatic amines ArNH_2 ($\text{Ar} = \text{Ph}$, 4- $\text{O}_2\text{NC}_6\text{H}_4$, 4- NCC_6H_4 , 2- $\text{MeO}_2\text{CC}_6\text{H}_4$, 2,6- $\text{Me}_2\text{C}_6\text{H}_3$) has been investigated under batch conditions (autoclave) in the presence of Y- and X-type zeolites. Operating at 120-150°C, highly selective mono-N-methylations are observed for anilines even when they are deactivated by either electronic effects or steric hindrance; typical selectivities for the formation of the corresponding mono-N-Me derivs. [$\text{ArNH}(\text{CH}_3)$] are in the range 92-98%, at a substrate conversion of 72-93%. A synergic effect between the reactivity of DMC (acting both as a methylating and as a reversible methoxycarbonylating agent) and the dual acid-base properties of zeolites is considered to be responsible for the unusually high selectivity observed; accordingly, a reaction mechanism is discussed, involving carbamates ($\text{ArNHCO}_2\text{CH}_3$) and N-methylcarbamates [$\text{ArN}(\text{CH}_3)\text{CO}_2\text{CH}_3$] as intermediates. The reaction is an example of a synthesis with low environmental impact: it couples the use of a non-toxic methylating agent (DMC, in place of the highly toxic Me halides or di-Me sulfate) with eco-friendly catalysts (zeolites) in a waste-free process.

CC 25-4 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)

ST amine arom methylation dimethyl carbonate zeolite

IT Methylation

(N-methylation of aromatic amines by di-Me carbonate over faujasite zeolites)

IT **Faujasite-type zeolites**
 RL: CAT (Catalyst use); USES (Uses)
 (N-methylation of aromatic amines by di-Me carbonate over faujasite zeolites)

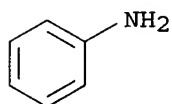
IT **Amines, reactions**
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (aromatic; N-methylation of aromatic amines by di-Me carbonate over faujasite zeolites)

IT 62-53-3, Benzenamine, reactions 87-62-7, 2,6-Dimethylaniline
 100-01-6, reactions 616-38-6, Dimethyl carbonate 619-45-4,
 Methyl 4-aminobenzoate 873-74-5, 4-Aminobenzonitrile
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (N-methylation of aromatic amines by di-Me carbonate over faujasite zeolites)

IT 85-91-6P 100-15-2P 100-23-2P 100-61-8P
 , preparation 121-69-7P, preparation 767-71-5P
 769-06-2P 1197-19-9P 1943-87-9P
 2603-10-3P 4714-62-9P 7143-42-2P
 10072-05-6P 20642-93-7P 28685-60-1P
 94563-11-8P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (N-methylation of aromatic amines by di-Me carbonate over faujasite zeolites)

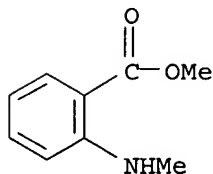
IT 62-53-3, Benzenamine, reactions
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (N-methylation of aromatic amines by di-Me carbonate over faujasite zeolites)

RN 62-53-3 CAPLUS
 CN Benzenamine (9CI) (CA INDEX NAME)

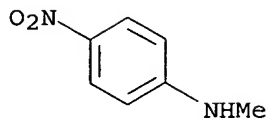


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 2603-10-3P 4714-62-9P 7143-42-2P
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 (N-methylation of aromatic amines by di-Me carbonate over faujasite zeolites)

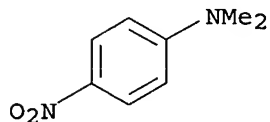
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RN 100-15-2 CAPLUS
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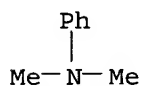
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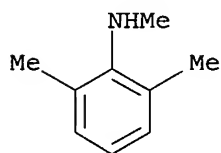
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CN Benzenamine, N-methyl- (9CI) (CA INDEX NAME)

Me-NH-Ph

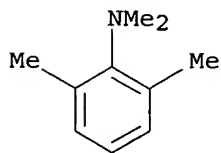
RN 121-69-7 CAPLUS
CN Benzenamine, N,N-dimethyl- (9CI) (CA INDEX NAME)



RN 767-71-5 CAPLUS
CN Benzenamine, N,2,6-trimethyl- (9CI) (CA INDEX NAME)

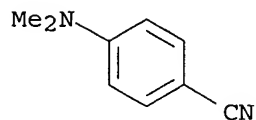


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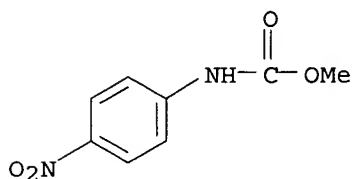
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CN Benzonitrile, 4-(dimethylamino)- (9CI) (CA INDEX NAME)



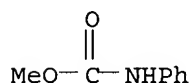
RN 1943-87-9 CAPLUS

CN Carbamic acid, (4-nitrophenyl)-, methyl ester (9CI) (CA INDEX NAME)



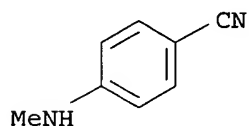
RN 2603-10-3 CAPLUS

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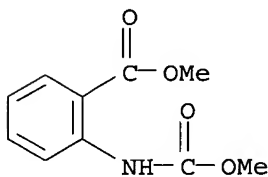
RN 4714-62-9 CAPLUS

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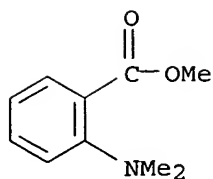
RN 7143-42-2 CAPLUS

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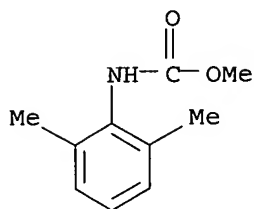
RN 10072-05-6 CAPLUS

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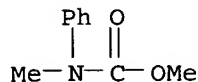
RN 20642-93-7 CAPLUS

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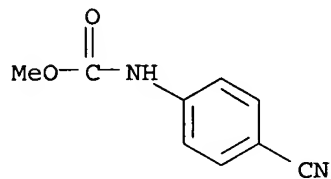
RN 28685-60-1 CAPLUS

CN Carbamic acid, methylphenyl-, methyl ester (9CI) (CA INDEX NAME)



RN 94563-11-8 CAPLUS

CN Carbamic acid, (4-cyanophenyl)-, methyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT:

24

THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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